



# **STIC Search Report**

## **Biotech-Chem Library**

**STIC Database Tracking Number: 138577**

**TO: Rei-Tsang Shiao**  
**Location: 5a10 / 5c18**  
**Tuesday, November 30, 2004**  
**Art Unit: 1626**  
**Phone: 272-0707**  
**Serial Number: 10 / 009407**

**From: Jan Delaval**  
**Location: Biotech-Chem Library**  
**Rem 1A51**  
**Phone: 272-2504**  
  
**jan.delaval@uspto.gov**

### **Search Notes**

John Delavel  
for search

Access DB# 138597

# SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Robert (Rety) Shiao Examiner #: 19521 Date: 1/23/04  
Art Unit: 1626 Phone Number: 2-0707 Serial Number: 10/009407  
Mail Box and Bldg/Room Location: 5A10/5C18 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

\*\*\*\*\*  
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

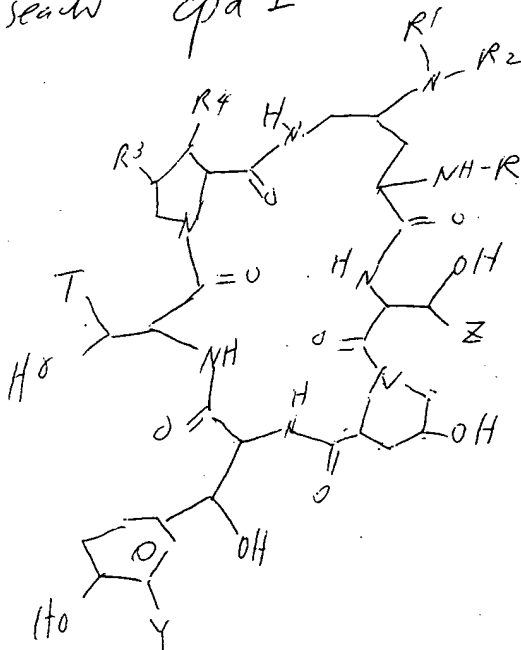
Title of Invention: Novel echinocandin derivative

Inventors (please provide full names): Bursson et al

Earliest Priority Filing Date: \_\_\_\_\_

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

I search cpd 2



1. R1 is -C(=O)-ary-hetero or  
-C(=O)-hetero or

2. R1, ~ R4 are sub.

3. T is sub

Y is sub

W is H or OH

Z is sub.

II process of making and Methods of use of cpd 2

## STAFF USE ONLY

Searcher: [Signature]  
Searcher Phone #: 22504  
Searcher Location: \_\_\_\_\_  
Date Searcher Picked Up: 1/30  
Date Completed: 1/30  
Searcher Prep. & Review Time: \_\_\_\_\_  
Critical Path Time: 10  
Online Time: + 15

## Type of Search

NA Sequence (#) \_\_\_\_\_  
AA Sequence (#) \_\_\_\_\_  
Structure (#) ☒ \_\_\_\_\_  
Bibliographic \_\_\_\_\_  
Litigation \_\_\_\_\_  
Fulltext \_\_\_\_\_  
Patent Family \_\_\_\_\_  
Other \_\_\_\_\_

## Vendors and cost where applicable

STN ☒ \_\_\_\_\_  
Dialog \_\_\_\_\_  
Questel/Orbit \_\_\_\_\_  
Dr.Link \_\_\_\_\_  
Lexis/Nexis \_\_\_\_\_  
Sequence Systems \_\_\_\_\_  
WWW/Internet \_\_\_\_\_  
Other (specify) \_\_\_\_\_

=> fil reg

FILE 'REGISTRY' ENTERED AT 14:25:36 ON 30 NOV 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 NOV 2004 HIGHEST RN 790189-55-8

DICTIONARY FILE UPDATES: 28 NOV 2004 HIGHEST RN 790189-55-8

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

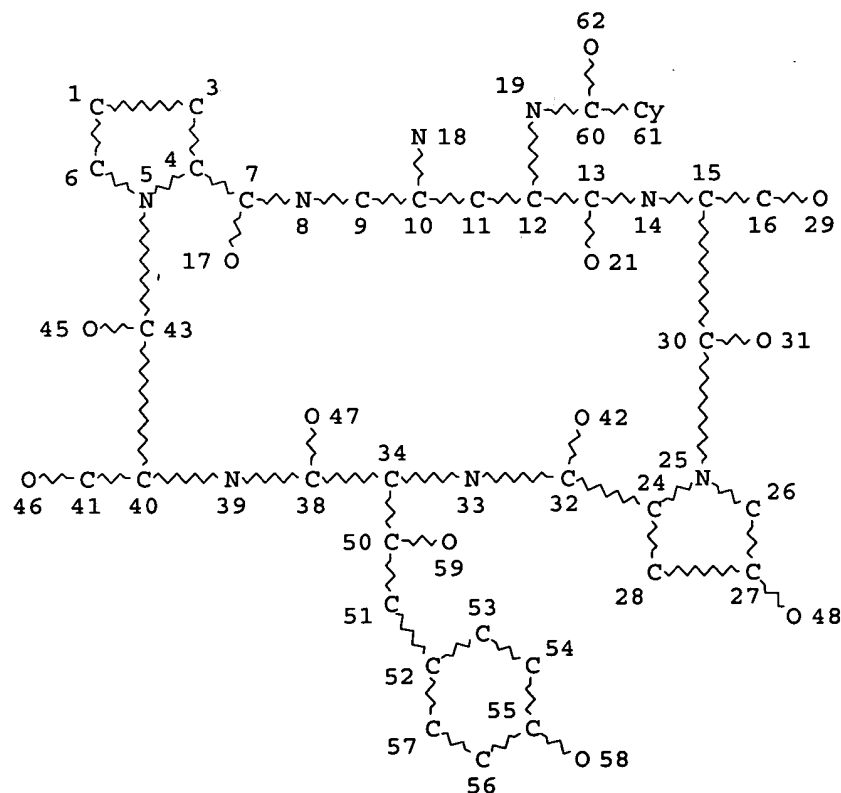
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d sta que l3

L1 STR



NODE ATTRIBUTES:

NSPEC IS RC AT 18

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 53

STEREO ATTRIBUTES: NONE

L3 55 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 97 ITERATIONS

55 ANSWERS

SEARCH TIME: 00.00.01

=> d his

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SET COST OFF

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L1 STR  
L2 3 S L1  
L3 55 S L1 FUL  
SAV TEMP L3 SHIAO009/A

FILE 'HCAOLD' ENTERED AT 14:22:39 ON 30 NOV 2004

L4 0 S L3

FILE 'HCAPLUS' ENTERED AT 14:22:43 ON 30 NOV 2004

L5 5 S L3  
L6 3 S L5 AND (CORBIER ? OR FAUVEAU ? OR PIETRE ? OR DISCHAMP ? OR S  
L7 1 S L5 AND AVENTI?/PA,CS  
L8 1 S L5 AND (US2002-009407# OR WO2000-FR1569 OR FR99-7252)/AP,PRN  
L9 2 S L7,L8  
L10 5 S L5-L9

FILE 'USPATFULL' ENTERED AT 14:25:21 ON 30 NOV 2004

L11 2 S L3

FILE 'REGISTRY' ENTERED AT 14:25:36 ON 30 NOV 2004

=> fil uspatfull

FILE 'USPATFULL' ENTERED AT 14:25:43 ON 30 NOV 2004

CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 30 Nov 2004 (20041130/PD)

FILE LAST UPDATED: 30 Nov 2004 (20041130/ED)

HIGHEST GRANTED PATENT NUMBER: US6826778

HIGHEST APPLICATION PUBLICATION NUMBER: US2004237163

CA INDEXING IS CURRENT THROUGH 30 Nov 2004 (20041130/UPCA)

ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 30 Nov 2004 (20041130/PD)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2004

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2004

>>> USPAT2 is now available. USPATFULL contains full text of the <<<  
>>> original, i.e., the earliest published granted patents or <<<  
>>> applications. USPAT2 contains full text of the latest US <<<  
>>> publications, starting in 2001, for the inventions covered in <<<  
>>> USPATFULL. A USPATFULL record contains not only the original <<<  
>>> published document but also a list of any subsequent <<<  
>>> publications. The publication number, patent kind code, and <<<  
>>> publication date for all the US publications for an invention <<<  
>>> are displayed in the PI (Patent Information) field of USPATFULL <<<  
>>> records and may be searched in standard search fields, e.g., /PN, <<<  
>>> /PK, etc. <<<

>>> USPATFULL and USPAT2 can be accessed and searched together <<<

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>>> through the new cluster USPATALL. Type FILE USPATALL to <<<
>>> enter this cluster. <<<
>>> <<<
>>> Use USPATALL when searching terms such as patent assignees, <<<
>>> classifications, or claims, that may potentially change from <<<
>>> the earliest to the latest publication. <<<
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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l11 bib abs hitrn fhitrstr tot

✓ L11 ANSWER 1 OF 2 USPATFULL on STN  
 AN 2004:95283 USPATFULL  
 TI Echinocandin derivatives, their method of preparation and their application as anti-fungal agents  
 IN Courtin, Olivier, Paris, FRANCE  
 Fauveau, Patrick, Livry Gargan, FRANCE  
 Markus, Astrid, Liederbach, GERMANY, FEDERAL REPUBLIC OF  
 Melon Manguer, Dominique, Montreuil, FRANCE  
 Michel, Jean-Marc, Compiègne, FRANCE  
 Schio, Laurent, Bondy, FRANCE  
 PA Aventis Pharma S.A. (non-U.S. corporation)  
 PI US 2004072737 A1 20040415  
 AI US 2003-666072 A1 20030919 (10)  
 RLI Division of Ser. No. US 2000-581451, filed on 24 Jul 2000, GRANTED, Pat. No. US 6677429 A 371 of International Ser. No. WO 1998-FR2671, filed on 9 Dec 1998, UNKNOWN  
 PRAI FR 1997-15628 19971210  
 FR 1998-13361 19981026  
 DT Utility  
 FS APPLICATION  
 LREP Charles A. Muserlian, c/o Muserlian, Lucas and Mercanti, 600 Third Avenue, New York, NY, 10016  
 CLMN Number of Claims: 27  
 ECL Exemplary Claim: 1  
 DRWN No Drawings  
 LN.CNT 733  
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.  
 AB Novel compounds of the formula ##STR1##

10666072

wherein the substituents are defined in the specification which are useful intermediates in the process to obtain compounds of Formula I which are useful as anti-fungal agents.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 227472-48-2P 227472-49-3P 227472-50-6P  
 227472-51-7P

(preparation of echinocandin derivs. as antifungal agents)

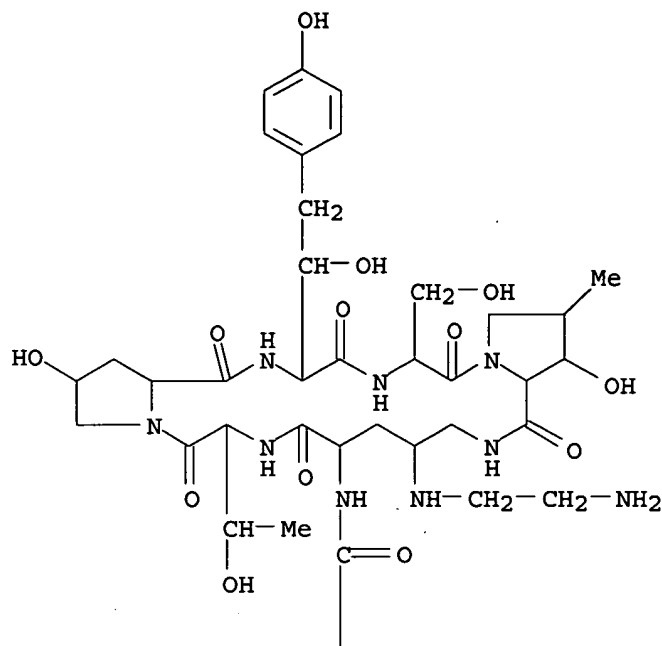
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(preparation of echinocandin derivs. as antifungal agents)

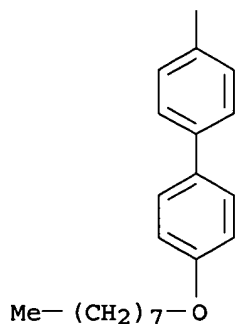
RN 227472-48-2 USPATFULL

CN Deoxymulundocandin, 1-[4-[(2-aminoethyl)amino]-N2-[[4'-(octyloxy)[1,1'-biphenyl]-4-yl]carbonyl]-L-ornithine]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



L11 ANSWER 2 OF 2 USPATFULL on STN  
 AN 2004:9645 USPATFULL  
 TI Echinocandin derivatives, preparation method and application as  
 anti-fungal agents  
 IN Courtin, Olivier, Paris, FRANCE  
 Fauveau, Patrick, Livry Gargan, FRANCE  
 Markus, Astrid, Liederbach, GERMANY, FEDERAL REPUBLIC OF  
 Melon Manguer, Dominique, Montreuil, FRANCE  
 Michel, Jean-Marc, Compiègne, FRANCE  
 Schio, Laurent, Bondy, FRANCE  
 PA Aventis Pharma S.A., FRANCE (non-U.S. corporation)  
 PI US 6677429 B1 20040113  
 WO 9929716 19990617  
 AI US 2000-581451 20000724 (9)  
 WO 1998-FR2671 19981209  
 PRAI FR 1997-15628 19971210

FR 1998-13361 19981026  
 DT Utility  
 FS GRANTED  
 EXNAM Primary Examiner: Low, Christopher S. F.; Assistant Examiner: Lukton, David  
 LREP Muserlian, Lucas and Mercanti  
 CLMN Number of Claims: 23  
 ECL Exemplary Claim: 1  
 DRWN 0 Drawing Figure(s); 0 Drawing Page(s)  
 LN.CNT 685

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A compound of Formula I in which R.sub.1 and R.sub.2=H, OH, alkyl optionally substituted, or NR.sub.1 forms with the carbon bearing NR.sub.1R.sub.2 a double bond and R.sub.2 is Xra, X being O, NH or N-alkyl and Ra being H, alkyl optionally substituted; R=a chain containing up to 10 carbon atoms, optionally comprising one or several heteroatoms, one or several heterocycles; T=H, CH.sub.2, CH.sub.2CONH.sub.2, CH.sub.2C.tbd., (CH.sub.2).sub.2NH.sub.2; Y=H, OH, halogen; W=H, OH; Z=H or CH.sub.3; said products have antifungal properties.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 227472-48-2P 227472-49-3P 227472-50-6P  
 227472-51-7P

(preparation of echinocandin derivs. as antifungal agents)

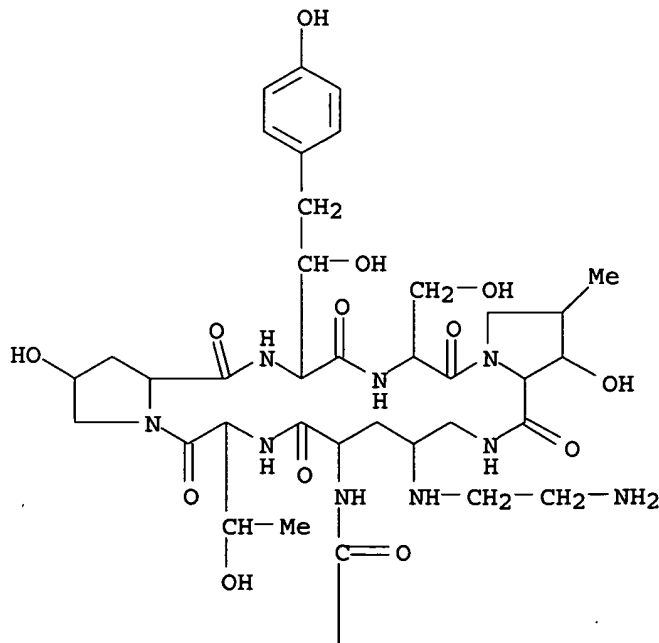
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(preparation of echinocandin derivs. as antifungal agents)

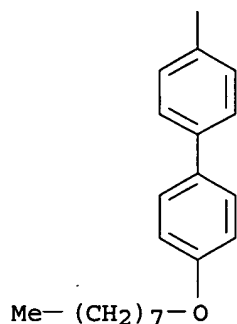
RN 227472-48-2 USPATFULL

CN Deoxymulundocandin, 1-[4-[(2-aminoethyl)amino]-N2-[[4'-(octyloxy)[1,1'-biphenyl]-4-yl]carbonyl]-L-ornithine]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



=&gt; fil hcaplus

FILE 'HCAPLUS' ENTERED AT 14:25:52 ON 30 NOV 2004

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FILE COVERS 1907 - 30 Nov 2004 VOL 141 ISS 23

FILE LAST UPDATED: 29 Nov 2004 (20041129/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=&gt; d l10 all fhitr tot

L10 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:475489 HCAPLUS

DN 139:53314

ED Entered STN: 22 Jun 2003

TI Procedure for preparation of echinocandin derivatives

IN Boffelli, Philippe; Brouillard, Agnes; Colladant, Colette; Droux, Serge; Elter, Michel; Ferroud, Didier; Lemaitre, Guy; Paladino, JosephPA Aventis Pharma S. A., Fr.

SO Fr. Demande, 36 pp.

CODEN: FRXXBL

DT Patent

LA French

IC ICM C07D487-14

ICS C07K007-56; A61K038-12; A61K031-4025; A61P031-10; C07D259-00; C07D207-12

CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 1

FAN.CNT 1

PATENT NO.

KIND

DATE

APPLICATION NO.

DATE



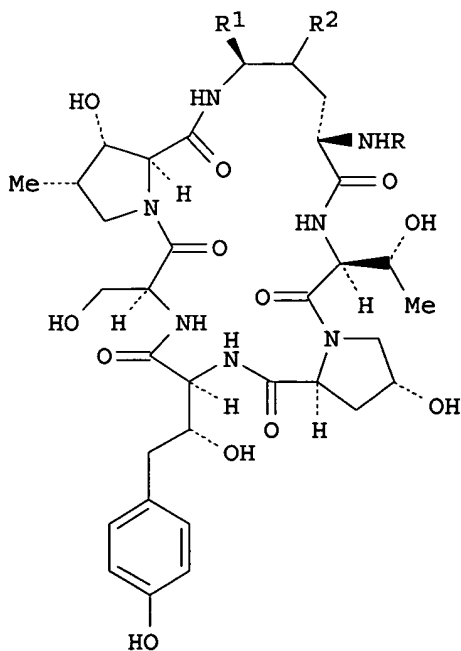
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PI  FR 2833596      A1    20030620    FR 2001-16230      20011214
    WO 2003054001   A2    20030703    WO 2002-FR4308     20021212
    WO 2003054001   A3    20040122
        W:  AE, AG, AL, AU, BA, BB, BR, BZ, CA, CN, CO, CR, CU, DM, DZ, EC,
            GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV,
            MA, MG, MK, MN, MX, NO, NZ, OM, PH, PL, RO, SC, SG, TN, TT, UA,
            US, UZ, VC, VN, YU, ZA
        RW:  GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
            FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ,
            CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
    EP 1456229      A2    20040915    EP 2002-805374     20021212
        R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
PRAI FR 2001-16230  A    20011214
    WO 2002-FR4308  W    20021212

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## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
FR 2833596	ICM	C07D487-14
	ICS	C07K007-56; A61K038-12; A61K031-4025; A61P031-10; C07D259-00; C07D207-12
FR 2833596	ECLA	C07K007/56
OS CASREACT 139:53314; MARPAT 139:53314		
GI		



I

AB Echinocandin derivs. I [R is an acyl group R1CO, where R1 is a chain (linear, branched, or cyclic) containing  $\geq 30$  carbon atoms containing one or more heteroatoms or heterocycles; R2 is H; R3 is NHCH2CH2NH2] were prepared for use as pharmaceuticals, in particular the dihydrochloride salts. The synthesis method involves acylation of I (R = H, R2, R3 = OH) by R1CO2H or an active ester, dehydration of the product or its mono-O-alkyl derivative, and reductive amination of the oxo derivative with

ethylenediamine in the presence of NaBH<sub>3</sub>CN and a Lewis acid or NaBH(O<sub>2</sub>CR')<sub>3</sub> (R'CO<sub>2</sub>H is Boc- or Cbz-L-Pro-OH). The product was obtained, mainly as one isomer, by using chromatog., crystallization, action of a base, and salification. In an example, the procedure was applied to the preparation of I (R<sub>1</sub> = 4-octylbiphenyl, R<sub>2</sub> is H; R<sub>3</sub> is NHCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub>) dihydrochloride.

ST echinocandin acyl aminoethylamino deriv prepn  
 IT Peptides, preparation  
 RL: IMF (Industrial manufacture); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (cyclic; preparation of echinocandin derivs.)

IT 545403-48-3P 545403-50-7P  
 RL: IMF (Industrial manufacture); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of echinocandin derivs.)

IT 310459-48-4P 545403-52-9P  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of echinocandin derivs.)

IT 545403-51-8P  
 RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation of echinocandin derivs.)

IT 545403-55-2P  
 RL: PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of echinocandin derivs.)

IT 107-15-3, Ethylenediamine, reactions 771-61-9, Pentafluorophenol 59748-18-4 227472-53-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of echinocandin derivs.)

IT 160430-95-5P 227472-54-0P 227472-55-1P 227472-60-8P 310459-54-2P 340020-20-4P 340131-54-6P 545403-46-1P 545403-47-2P 545403-49-4P 545403-53-0P 545403-54-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of echinocandin derivs.)

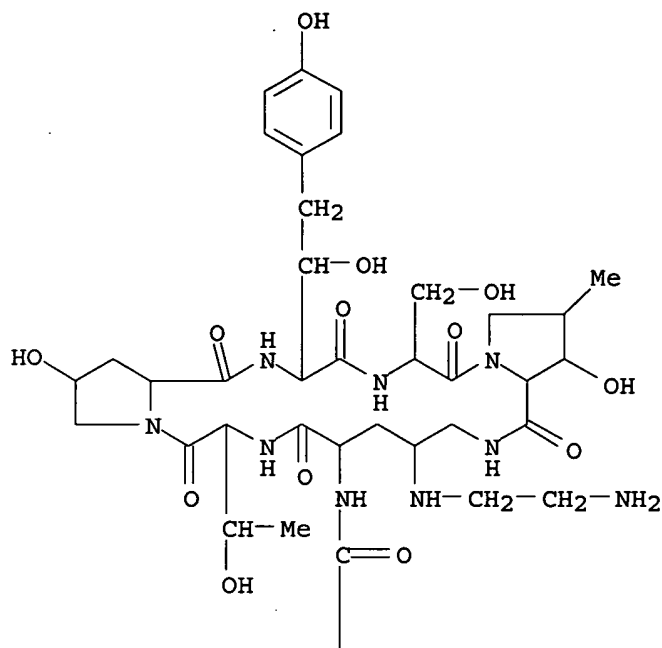
IT 10377-58-9, Magnesium iodide 40635-66-3, α Acetoxyisobutyryl chloride 41473-62-5 80934-48-1 546086-00-4  
 RL: RGT (Reagent); RACT (Reactant or reagent)  
 (preparation of echinocandin derivs.)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 RE  
 (1) Aventis Pharma GmbH; WO 0107468 A 2001 HCAPLUS  
 (2) Markus, A; WO 9929716 A 1999 HCAPLUS

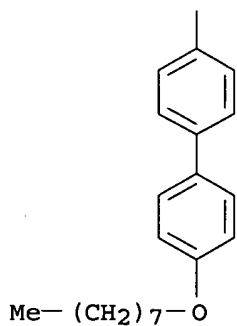
IT 545403-48-3P  
 RL: IMF (Industrial manufacture); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of echinocandin derivs.)

RN 545403-48-3 HCAPLUS  
 CN Deoxymulundocandin, 1-[(4R)-4-[(2-aminoethyl)amino]-N2-[[4'-(octyloxy)[1,1'-biphenyl]-4-yl]carbonyl]-L-ornithine]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



L10 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2000:881187 HCAPLUS  
 DN 134:17732  
 ED Entered STN: 15 Dec 2000  
 TI Novel echinocandin derivatives, method for preparing same and use as  
 antifungal agents  
 IN Corbier, Alain; Fauveau, Patrick;  
 Pietre-Dischamp, Nathalie; Schio, Laurent; Vicat,  
 Pascale  
 PA Hoechst Marion Roussel, Fr.  
 SO PCT Int. Appl., 34 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA French  
 IC ICM C07K007-56  
 ICS A61K038-12; A61P031-10

CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 1, 10, 63

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000075178	A1	20001214	WO 2000-FR1569	20000608 <--
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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	FR 2794747	B1	20040416		
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	EP 1189932	A1	20020327	EP 2000-940456	20000608 <--
	EP 1189932	B1	20030521		
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	JP 2003504309	T2	20030204	JP 2001-502459	20000608 <--
	AT 240971	E	20030615	AT 2000-940456	20000608 <--
	PT 1189932	T	20030930	PT 2000-940456	20000608 <--
	ES 2194744	T3	20031201	ES 2000-940456	20000608 <--
PRAI	FR 1999-7252	A	19990609	<--	
	WO 2000-FR1569	W	20000608	<--	

CLASS

	PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
	WO 2000075178	ICM	C07K007-56
		ICS	A61K038-12; A61P031-10
	FR 2794747	ECLA	C07K007/56
OS	CASREACT 134:17732; MARPAT 134:17732		
GI			

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention concerns cyclic peptides I wherein: R = chain containing up to 30 carbon atoms, optionally containing one or several heteroatoms, one or several heterocycles; either R1 and R2 = H, OH, alkyl optionally substituted, or NR1 forms with the carbon bearing NR1R2 a double bond and R2 is XRa, X being O, NH or N-alkyl and Ra being H, alkyl optionally substituted; R3 = H, OH, CH3; R4 = H, OH; T = H, CH3, CH2CONH2, CH2CN, (CH2)2NH2; Y = H, OH, halogen, OSO3H; W = H, OH; Z = H or CH3. The products of formula I have antifungal properties. Thus, trans-1-[4-[(2-aminocyclo-hexyl)amino]-N2-[[4-[5-[4-(pentyloxy)phenyl]-3-isoxazolyl]phenyl]carbonyl]-L-ornithine]-4-[4-(4-hydroxyphenyl)-L-threonine]-5-L-serine-echinocandin B trifluoroacetate was prepared and tested for its inhibition of glucan synthase of *Candida albicans*.

ST echinocandin cyclic peptide prepn antifungal glucan synthase inhibitor

IT Peptides, preparation

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(cyclic; novel echinocandin derivs. method for preparing same and use as glucan synthase inhibitors and antifungal agents)

IT Fungicides

(novel echinocandin derivs. method for preparing same and use as glucan synthase inhibitors and antifungal agents)

IT 9027-19-4, Glucan synthase

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(Candida albicans; novel echinocandin derivs. method for preparing same and use as glucan synthase inhibitors and antifungal agents)

IT 310459-08-6P 310459-11-1P 310459-20-2P  
310459-23-5P 310459-27-9P 310459-30-4P  
310459-33-7P 310459-36-0P 310459-39-3P  
310459-42-8P 310459-49-5P 310459-52-0P  
310459-58-6P 310459-61-1P 310459-67-7P  
310459-70-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(novel echinocandin derivs. method for preparing same and use as glucan synthase inhibitors and antifungal agents)

IT 15967-72-3, (S)-Propane-1,2-diamine 20439-47-8 21436-03-3  
38734-69-9, Ethylenediamine diacetate 138626-63-8, Deoxymulundocandin  
179165-34-5 310459-15-5 340130-90-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(novel echinocandin derivs. method for preparing same and use as glucan synthase inhibitors and antifungal agents)

IT 227472-53-9P 310459-13-3P 310459-17-7P 310459-44-0P 310459-46-2P  
310459-54-2P 340131-54-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(novel echinocandin derivs. method for preparing same and use as glucan synthase inhibitors and antifungal agents)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Fujisawa Pharmaceutical Co; EP 0644199 A 1995 HCAPLUS
- (2) Lilly Co Eli; EP 0736541 A 1996 HCAPLUS
- (3) Markus, A; WO 9929716 A 1999 HCAPLUS
- (4) Merck & Co Inc; WO 9613272 A 1996 HCAPLUS
- (5) Ohki, H; WO 9823637 A 1998 HCAPLUS

IT 310459-08-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(novel echinocandin derivs. method for preparing same and use as glucan synthase inhibitors and antifungal agents)

RN 310459-08-6 HCAPLUS

CN Deoxymulundocandin, 1-[(4R)-4-[(2-aminoethyl)amino]-N2-[4-[5-[4-(pentyloxy)phenyl]-3-isoxazolyl]benzoyl]-L-ornithine]-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

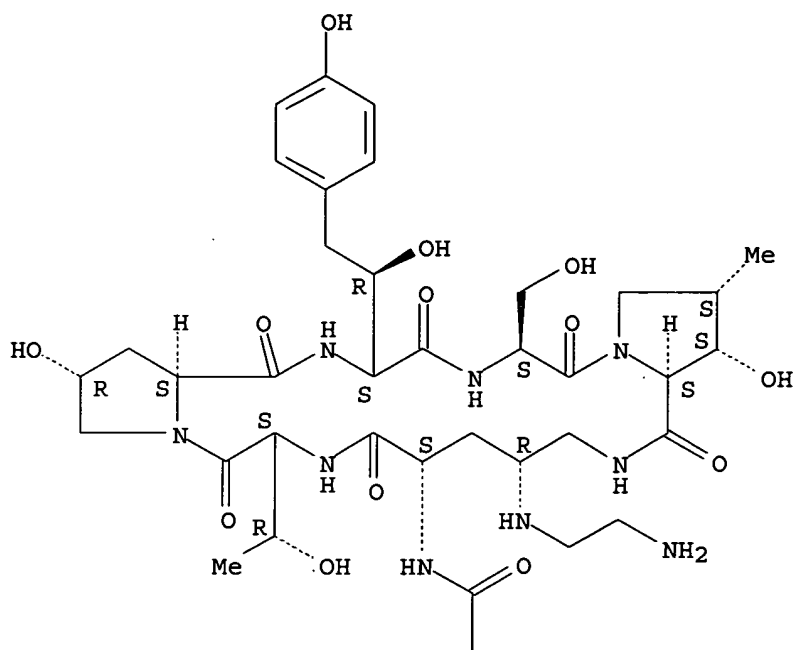
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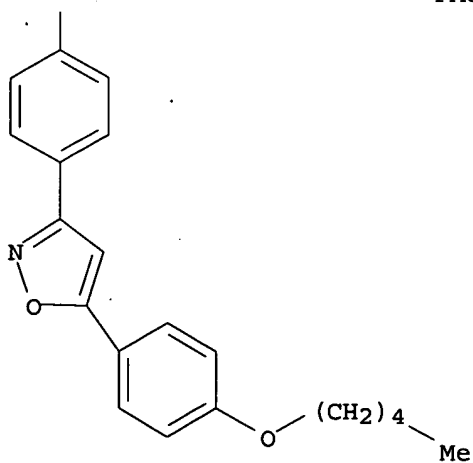
CMF C56 H74 N10 O15

Absolute stereochemistry.

PAGE 1-A



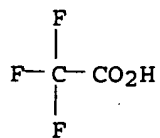
PAGE 2-A



CM 2

CRN 76-05-1

CMF C2 H F3 O2



B10 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2000:881186 HCAPLUS  
 DN 134:17731  
 ED Entered STN: 15 Dec 2000  
 TI Echinocandin derivatives, method for preparing same and application as  
 glucan synthase inhibitors and antifungal agents  
 IN Fauveau, Patrick; Hawser, Stephen; Lebourg, Gilles; Schio,  
 Laurent  
 PA Hoechst Marion Roussel, Fr.  
 SO PCT Int. Appl., 24 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA French  
 IC ICM C07K007-56  
 ICS A61K038-12; A61P031-10  
 CC 34-3 (Amino Acids, Peptides, and Proteins)  
 Section cross-reference(s): 7, 10, 63  
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000075177	A1	20001214	WO 2000-FR1568	20000608
W: AE, AG, AL, AU, BA, BB, BG, BR, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, MZ, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2794746	A1	20001215	FR 1999-7251	19990609
FR 2794746	B1	20021206		
CA 2376025	AA	20001214	CA 2000-2376025	20000608
EP 1189933	A1	20020327	EP 2000-942169	20000608
EP 1189933	B1	20030409		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2003501441	T2	20030114	JP 2001-502458	20000608
AT 236928	E	20030415	AT 2000-942169	20000608
PT 1189933	T	20030829	PT 2000-942169	20000608
ES 2192533	T3	20031016	ES 2000-942169	20000608
PRAI FR 1999-7251	A	19990609		
WO 2000-FR1568	W	20000608		

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2000075177	ICM	C07K007-56
	ICS	A61K038-12; A61P031-10
FR 2794746	ECLA	C07K007/56
OS	CASREACT	134:17731; MARPAT 134:17731
GI		

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention concerns in all possible isomeric forms as well as their  
 mixts., cyclic peptides I wherein: R represents a linear, branched or  
 cyclic chain; either R1 represents H or CH3 and R2 represents cyclohexyl  
 substituted by an amine, cyanoalkyl ; or R1 and R2 form with the nitrogen  
 which bears them a cycle with 3, 4 or 5 carbons optionally substituted by  
 an amine; R3 represents hydrogen, Me or hydroxyl; R4 represents hydrogen

or hydroxyl; T represents hydrogen, Me, CH<sub>2</sub>CONH<sub>2</sub>, CH<sub>2</sub>CN, a (CH<sub>2</sub>)<sub>2</sub>NH<sub>2</sub> or (CH<sub>2</sub>)<sub>2</sub>Nalk+X- radical, X being halogen and alk an alkyl radical; Y represents hydrogen, hydroxyl, halogen or OSO<sub>3</sub>H; W represents H or OH; Z represents H, CH<sub>3</sub>. The compds. of formula I have antifungal properties. Thus, . Trans 1-[4-[(2-aminocyclohexyl)amino]-N<sub>2</sub>-[[4'-(pentyloxy)[1,1':4',1''terphenyl]-4-yl]carbonyl]-L-ornithine]-4-[4-(4-hydroxyphenyl)-L-threonine]-5-L-serine-echinocandine B trifluoroacetate was prepared and tested for its inhibition of glucan synthase of *Candida albicans* and of the enzyme prepared from *Aspergillus fumigatus*.

ST echinocandin cyclic peptide prepn antifungal glucan synthase inhibitor  
 IT Peptides, preparation  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (cyclic; echinocandin derivs., method for preparing same and application as glucan synthase inhibitors and antifungal agents)  
 IT *Aspergillus fumigatus*  
 Fungicides  
 (echinocandin derivs., method for preparing same and application as glucan synthase inhibitors and antifungal agents)  
 IT 9027-19-4, Glucan synthase  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (Candida albicans; echinocandin derivs., method for preparing same and application as glucan synthase inhibitors and antifungal agents)  
 IT 310461-86-0P 310461-89-3P 310461-95-1P  
 310461-97-3P 310461-99-5P 310462-01-2P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (echinocandin derivs., method for preparing same and application as glucan synthase inhibitors and antifungal agents)  
 IT 538-75-0, N,N'-Dicyclohexylcarbodiimide 771-61-9, 2,3,4,5,6-Pentafluorophenol 5805-57-2, 2-(Aminomethyl)benzimidazole 19777-66-3  
 20439-47-8 59748-18-4 138626-63-8, Deoxymulundocandin 227472-60-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (echinocandin derivs., method for preparing same and application as glucan synthase inhibitors and antifungal agents)  
 IT 160430-95-5P 227472-53-9P 227472-54-0P 227472-55-1P 340020-20-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (echinocandin derivs., method for preparing same and application as glucan synthase inhibitors and antifungal agents)  
 RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 RE  
 (1) Markus, A; WO 9929716 A 1999 HCAPLUS  
 (2) Merck & Co Inc; WO 9613272 A 1996 HCAPLUS  
 IT 310461-86-0P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (echinocandin derivs., method for preparing same and application as glucan synthase inhibitors and antifungal agents)  
 RN 310461-86-0 HCAPLUS  
 CN Deoxymulundocandin, 1-[(4R)-4-[(2S)-2-aminopropyl]amino]-N<sub>2</sub>-[[4'-(octyloxy)[1,1'-biphenyl]-4-yl]carbonyl]-L-ornithine]-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

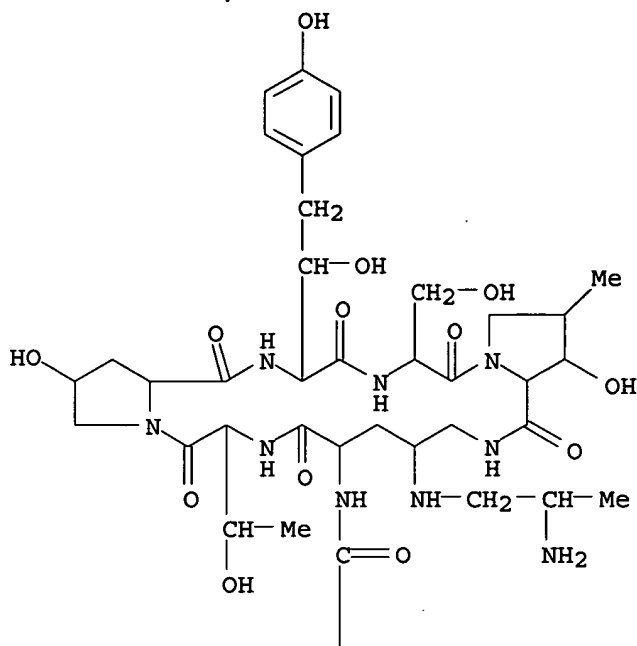
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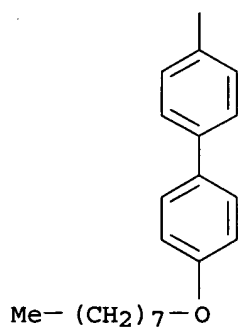
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PAGE 1-A



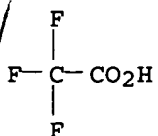
PAGE 2-A



CM 2

CRN 76-05-1

CMF C2 H F3 O2



DN 132:308664  
 ED Entered STN: 05 May 2000  
 TI Photochemical process for conversion of the 1,2-diol moiety of an echinocandin compound to the 1-deoxy-2-keto analog  
 IN Hitchcock, Stephen Andrew; Gregory, George Stuart  
 PA Eli Lilly and Company, USA  
 SO PCT Int. Appl., 28 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07B041-06  
 ICS C07K007-56  
 CC 34-3 (Amino Acids, Peptides, and Proteins)  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000024694	A1	20000504	WO 1999-US25301	19991027
	W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
PRAI	US 1998-105936P	P	19981028		

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2000024694	ICM	C07B041-06
	ICS	C07K007-56

OS CASREACT 132:308664; MARPAT 132:308664

AB A method for converting an epoxy or hydroxy moiety to a 1-deoxy-2-keto moiety is described which includes: (1) reacting a compound having an epoxy or hydroxy moiety with a thiophenol and (2) irradiating the 1-phenylthio-2-hydroxy moiety with UV or near-UV radiation to convert the 1-phenylsulfide-2-hydroxy moiety to a 1-deoxy-2-keto moiety. The process was used to modify the cyclic peptide ring system of an echinocandin-type compound containing a 1,2-diol moiety to produce new keto analogs.

ST echinocandin diol conversion deoxy keto analog; keto analog echinocandin prepn

IT Peptides, preparation

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (cyclic; photochem. process for conversion of diol moiety of an echinocandin compound to 1-deoxy-2-keto analog)

IT 266317-26-4P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (photochem. process for conversion of diol moiety of an echinocandin compound to 1-deoxy-2-keto analog)

IT 266317-27-5P 266317-28-6P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (photochem. process for conversion of diol moiety of an echinocandin compound to 1-deoxy-2-keto analog)

IT 119-26-6, 2,4-Dinitrophenylhydrazine 1099-45-2, Ethyl triphenylphosphoranylideneacetate 37972-89-7, Benzenethiol, 2-iodo-166663-25-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(photochem. process for conversion of diol moiety of an echinocandin compound to 1-deoxy-2-keto analog)

IT 266317-25-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(photochem. process for conversion of diol moiety of an echinocandin compound to 1-deoxy-2-keto analog)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Hoechst Marion Roussel; WO 9929716 A 1999 HCAPLUS
- (2) Merck; EP 0448353 A 1991 HCAPLUS
- (3) Merck; WO 9624613 A 1996 HCAPLUS
- (4) Piva, O; TETRAHEDRON LETTERS 1992, V33(18), P2459 HCAPLUS

IT 266317-27-5P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

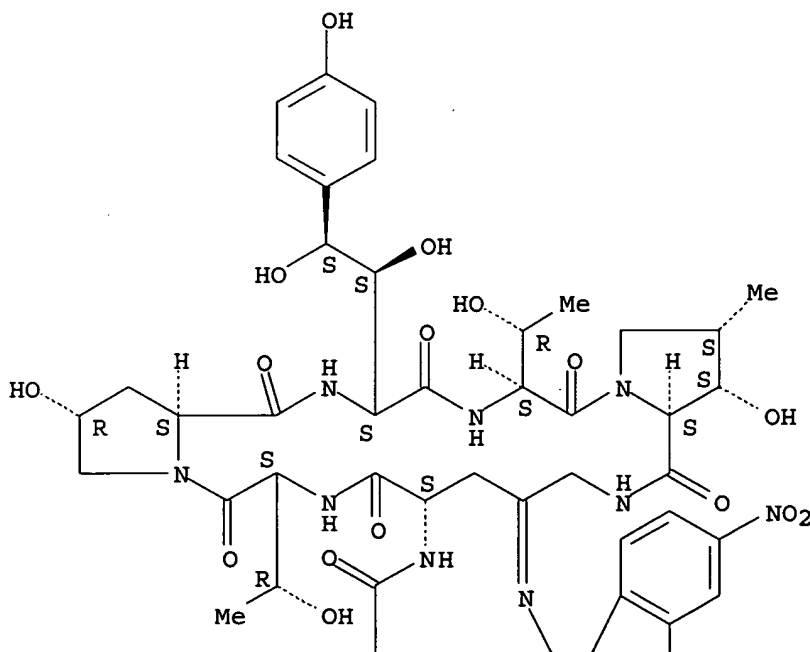
(photochem. process for conversion of diol moiety of an echinocandin compound to 1-deoxy-2-keto analog)

RN 266317-27-5 HCAPLUS

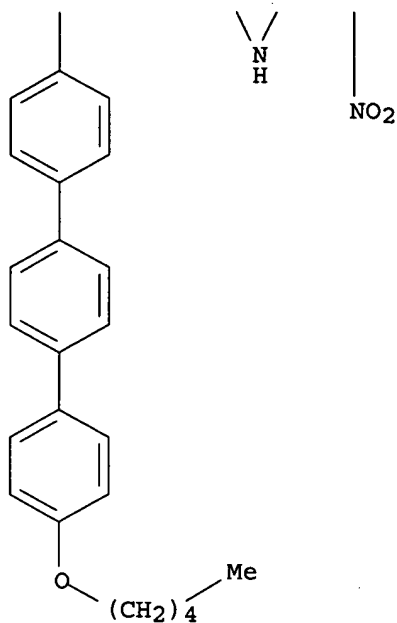
CN Echinocandin B, 1-[4-[(2,4-dinitrophenyl)hydrazono]-N2-[[4'-(pentyloxy)[1,1':4',1''-terphenyl]-4-yl]carbonyl]-L-ornithine] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry unknown.

PAGE 1-A



PAGE 2-A



L10 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1999:390418 HCAPLUS  
 DN 131:45105  
 ED Entered STN: 24 Jun 1999  
 TI Preparation of Echinocandin B derivatives as antifungal agents  
 IN Courtin, Olivier; Fauveau, Patrick; Markus, Astrid; Melon  
 Manguer, Dominique; Michel, Jean-Marc; Schio, Laurent  
 PA Hoechst Marion Roussel, Fr.  
 SO PCT Int. Appl., 46 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA French  
 IC ICM C07K007-56  
 ICS A61K038-12  
 CC 34-3 (Amino Acids, Peptides, and Proteins)  
 Section cross-reference(s): 1  
 FAN.CNT 1

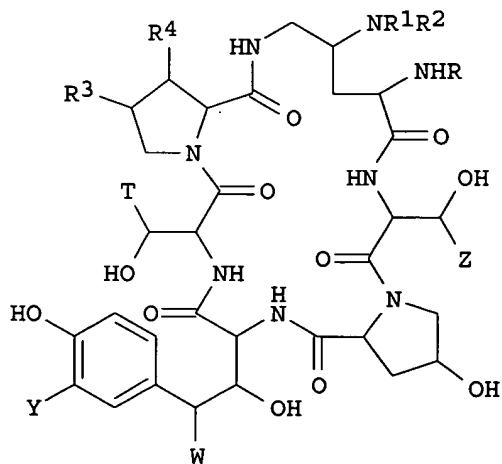
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9929716	A1	19990617	WO 1998-FR2671	19981209
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2772028	A1	19990611	FR 1997-15628	19971210
FR 2772028	B1	20000204		
FR 2784993	A1	20000428	FR 1998-13361	19981026
FR 2784993	B1	20021031		
ZA 9811158	A	19991207	ZA 1998-11158	19981207
CA 2311295	AA	19990617	CA 1998-2311295	19981209
AU 9915659	A1	19990628	AU 1999-15659	19981209
AU 755033	B2	20021128		
EP 1036090	A1	20000920	EP 1998-959935	19981209

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE,  
SI, LT, LV, FI, RO

BR 9813531	A	20001010	BR 1998-13531	19981209
TR 200001655	T2	20001121	TR 2000-200001655	19981209
EE 200000336	A	20010815	EE 2000-200000336	19981209
JP 2001525421	T2	20011211	JP 2000-524307	19981209
NZ 504614	A	20021220	NZ 1998-504614	19981209
TW 446541	B	20010721	TW 1998-87121185	19990122
BG 104494	A	20010131	BG 2000-104494	20000531
NO 2000002959	A	20000809	NO 2000-2959	20000609
HR 2000000384	A1	20001031	HR 2000-384	20000609
US <del>6677429</del>	B1	20040113	US 2000-581451	20000724
US 2004072737	A1	20040415	US 2003-666072	20030919
PRAI FR 1997-15628	A	19971210		
FR 1998-13361	A	19981026		
WO 1998-FR2671	W	19981209		
US 2000-581451	A3	20000724		

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9929716	ICM	C07K007-56
	ICS	A61K038-12
WO 9929716	ECLA	C07K007/56
FR 2772028	ECLA	C07K007/56
FR 2784993	ECLA	C07K007/56
US 6677429	ECLA	C07K007/56
US 2004072737	ECLA	C07K007/56
OS MARPAT 131:45105		
GI		



I

AB The title compds. I (R1, R2 = H, OH, (substituted) alkyl, NR1 forms with the carbon bearing NR1R2 a double bond and R2 = MP; M = O, NH, alkylamino; P = H, (substituted) alkyl; R3 = H, OH, CH3; R4 = H, OH; R = linear or branched chain up to 30 carbon atoms optionally substituted with heteroatoms, aryls or heterocycles; T = H, CH3, CH2CONH2, CH2C.tplbond.N, (CH2)2NH2; Y = H, OH, halogen; W = H, OH; Z = H, CH3) were prepared as antifungal agents (no data given). For example, 1-[(4R,5R)-4,5-dihydroxy-N2-(12-methyltetradecanoyl)-L-ornithine]-4-[4-(4-hydroxyphenyl)-L-threonine]-5-L-serine-echinocandin B was treated with trimethylsilyl iodide and sodium thiosulfate in succession to give the intermediate

1-[N2-(12-methyltetradecanoyl)-4-oxo-L-ornithine]-4-[4-(4-hydroxyphenyl)-L-threonine]-5-L-serine-echinocandin B in 62% yield. This intermediate, when treated with 2-(dimethylamino)ethylamine, gave the final product I [NR1R2 = NHCH2CH2NMe2, R = CO(CH2)10CH(CH3)CH2CH3, Z = CH3, W = Y = T = H, R3 = CH3, R4 = OH] as a mixture of isomers, which were, then, separated via HPLC.

ST echinocandin B deriv prepn antifungal agent

IT Fungicides

(preparation of echinocandin derivs. as antifungal agents)

IT 227472-27-7P 227472-67-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation of echinocandin derivs. as antifungal agents)

IT 227472-29-9P 227472-31-3P 227472-33-5P 227472-34-6P 227472-35-7P  
227472-37-9P 227472-38-0P 227472-39-1P 227472-40-4P 227472-41-5P  
227472-42-6P 227472-43-7P 227472-45-9P 227472-47-1P

227472-48-2P 227472-49-3P 227472-50-6P

227472-51-7P 227472-62-0P 227472-63-1P 227472-64-2P

227472-66-4P 227472-68-6P 227472-70-0P 227472-72-2P 227472-73-3P

227472-74-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of echinocandin derivs. as antifungal agents)

IT 107-15-3, 1,2-Ethanediamine, reactions 108-00-9, 2-  
(Dimethylamino)ethylamine 109-76-2, 1,3-Diaminopropane 1937-19-5  
3279-95-6 55959-84-7 59748-18-4 65920-18-5 227472-53-9  
227472-57-3 227614-36-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of echinocandin derivs. as antifungal agents)

IT 138626-63-8P, Deoxymulundocandin 160430-95-5P 227472-52-8P  
227472-54-0P 227472-55-1P 227472-56-2P 227472-58-4P 227472-59-5P  
227472-60-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of echinocandin derivs. as antifungal agents)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Balkovec, J; WO 9608267 A 1991 HCAPLUS
- (2) Balkovec, J; WO 9613272 A 1996 HCAPLUS
- (3) Bouffard, F; WO 9622784 A 1996 HCAPLUS
- (4) Lilly Co E; EP 0561639 A 1993 HCAPLUS
- (5) Lilly Co E; EP 0736541 A 1996 HCAPLUS
- (6) Merck & Co Inc; GB 2241955 A 1991 HCAPLUS

IT 227472-48-2P

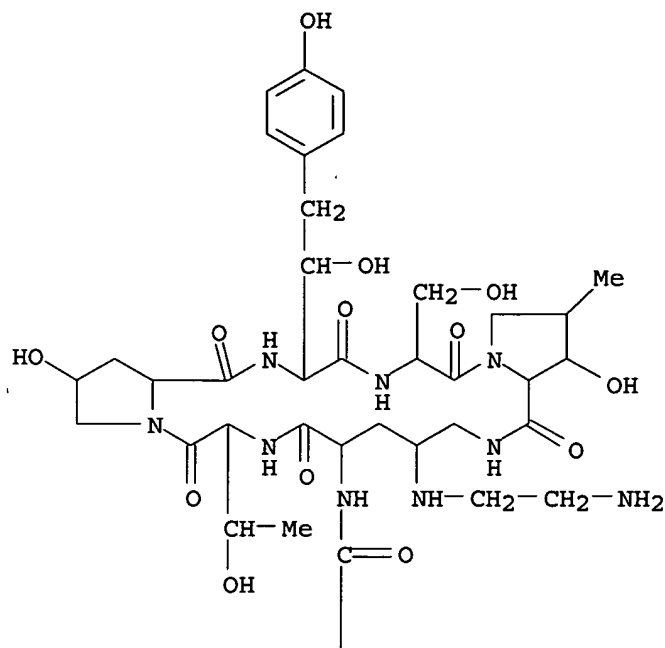
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of echinocandin derivs. as antifungal agents)

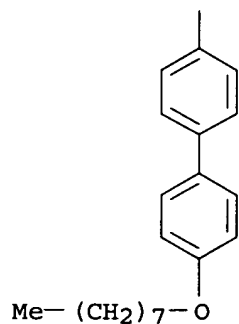
RN 227472-48-2 HCAPLUS

CN Deoxymulundocandin, 1-[4-[(2-aminoethyl)amino]-N2-[[4'-(octyloxy)[1,1'-biphenyl]-4-yl]carbonyl]-L-ornithine]- (9CI) (CA INDEX NAME)

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DICTIONARY FILE UPDATES: 28 NOV 2004 HIGHEST RN 790189-55-8

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conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

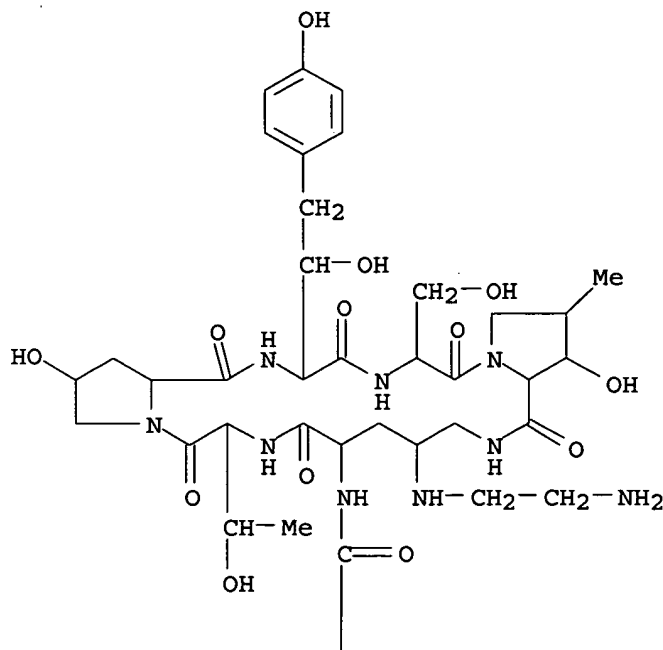
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RN 754974-66-8 REGISTRY  
CN Deoxymulundocandin, 1-[(4S)-4-[(2-aminoethyl)amino]-N2-[[4'-(octyloxy)[1,1'-biphenyl]-4-yl]carbonyl]-L-ornithine]- (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
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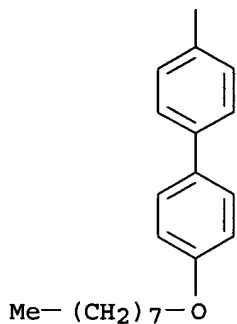
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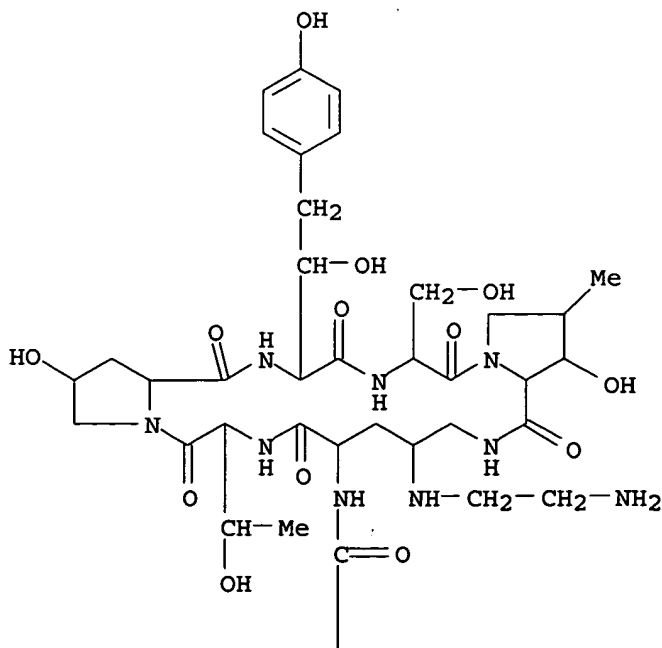


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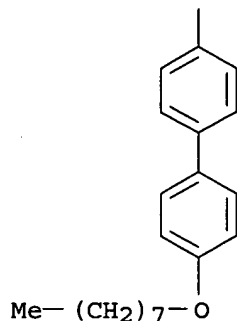
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 DT.CA Caplus document type: Patent  
 RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)  
 CRN (754974-66-8)

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

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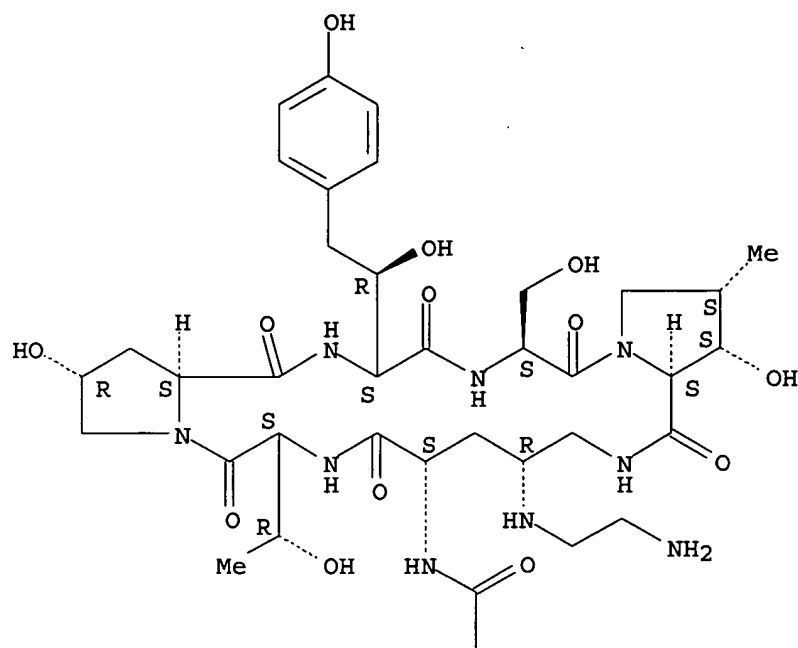
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L3 ANSWER 3 OF 55 REGISTRY COPYRIGHT 2004 ACS on STN  
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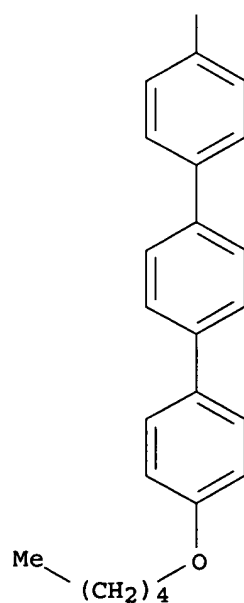
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Absolute stereochemistry.

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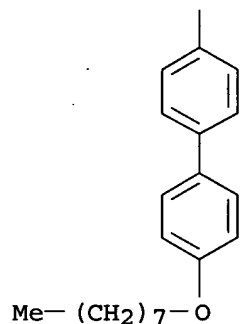
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REFERENCE 1: 139:53314

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RN 545403-50-7 REGISTRY  
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FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C56 H79 N9 O14 . 2 C2 H F3 O2  
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RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

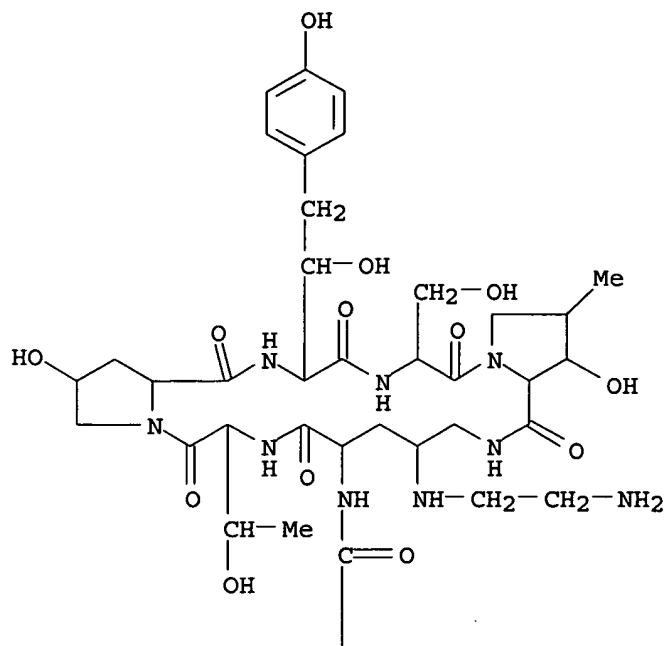
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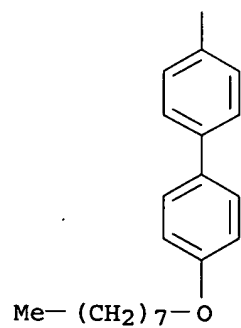
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CMF C56 H79 N9 O14

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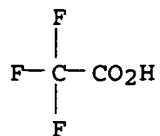
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CRN 76-05-1

CMF C2 H F3 O2



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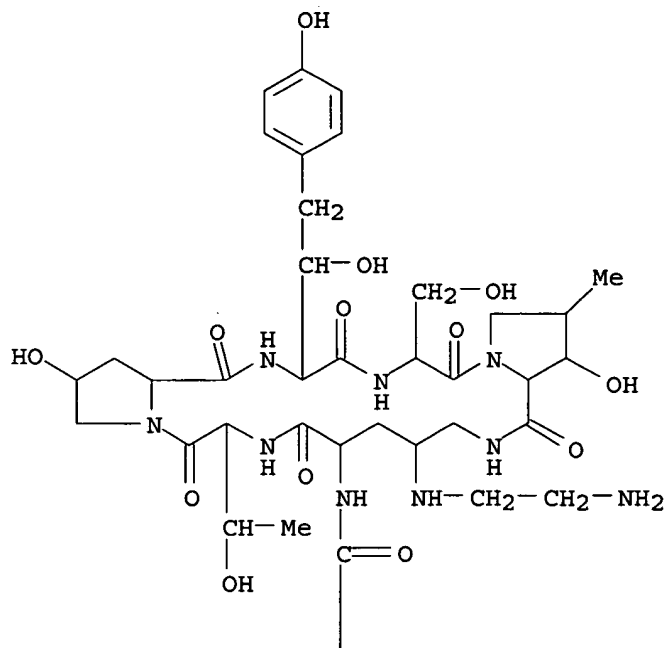
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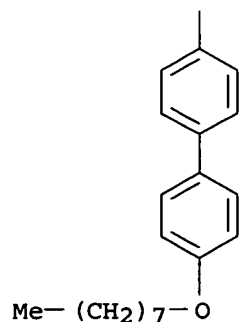
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 FS PROTEIN SEQUENCE; STEREOSEARCH  
 MF C56 H79 N9 O14  
 CI COM  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT  
 DT.CA Caplus document type: Patent  
 RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

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## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:53314

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RN 310462-01-2 REGISTRY  
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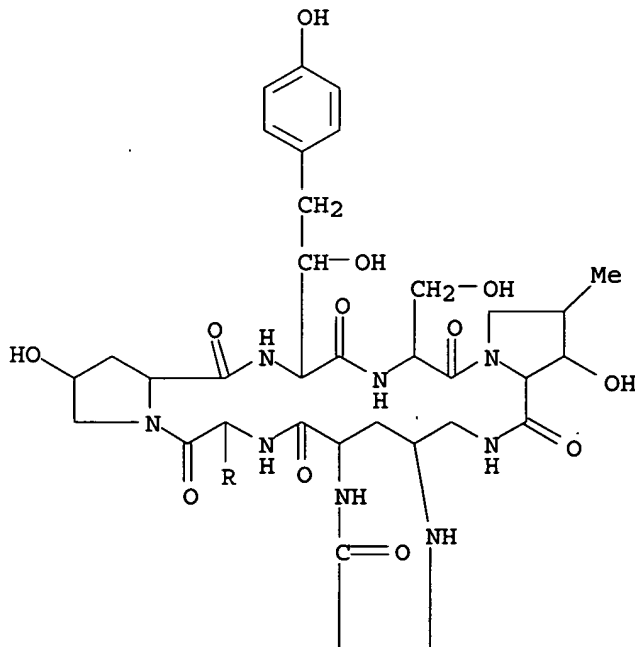
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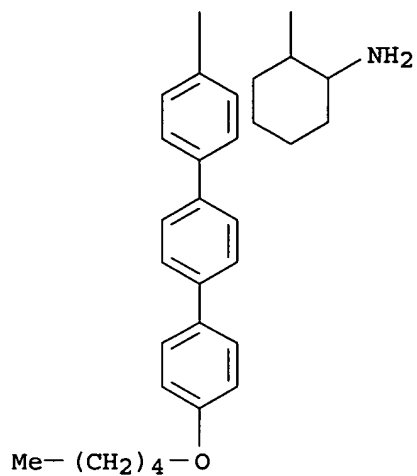
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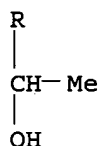




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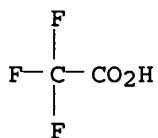
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CMF C2 H F3 O2



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REFERENCE 1: 134:17731

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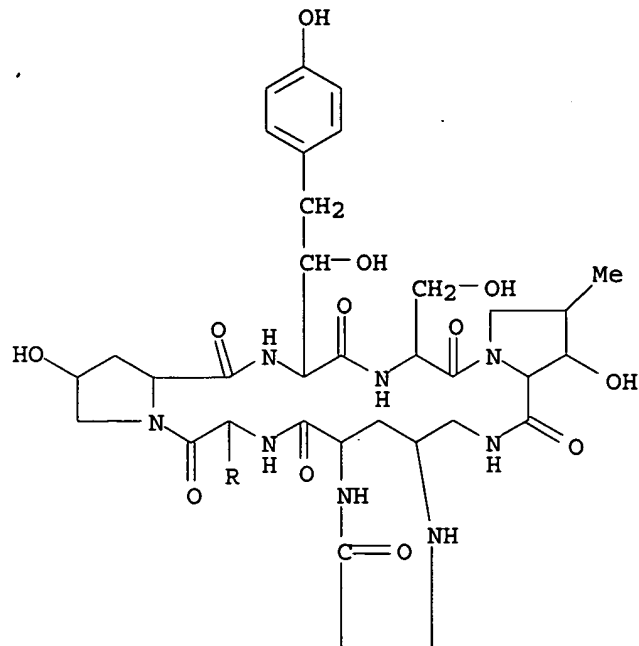
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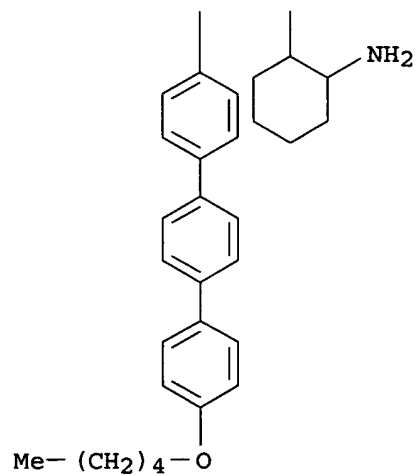
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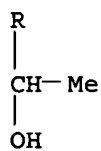
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CN Deoxymulundocandin, 1-[(4R)-4-[[[(1R,2R)-2-aminocyclohexyl]amino]-N2-[[4''-(pentyloxy)[1,1':4',1''-terphenyl]-4-yl]carbonyl]-L-ornithine]-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C63 H83 N9 O14 . x C2 H F3 O2  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT  
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RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

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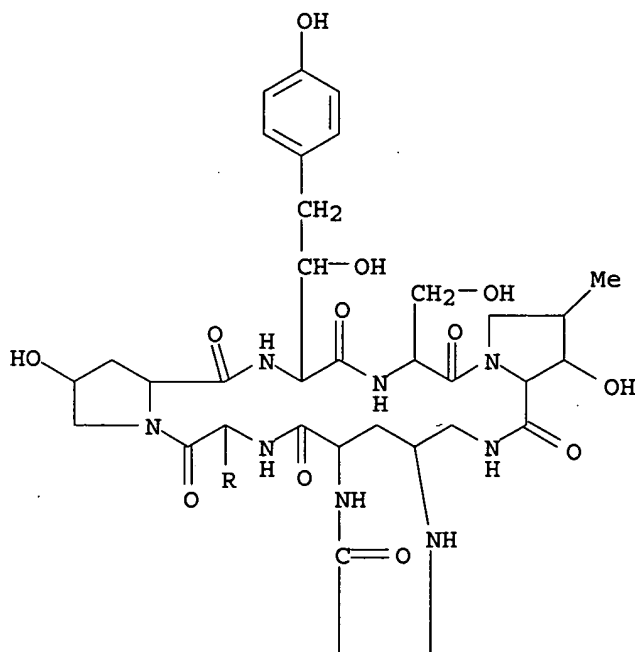
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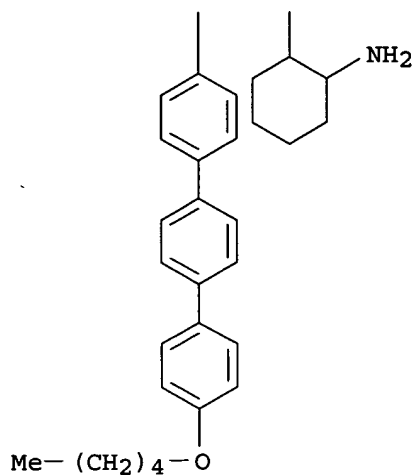
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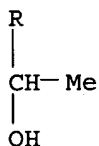
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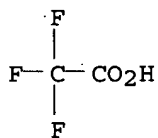
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CRN 76-05-1

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1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:17731

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RN 310461-98-4 REGISTRY

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FS PROTEIN SEQUENCE; STEREOSEARCH

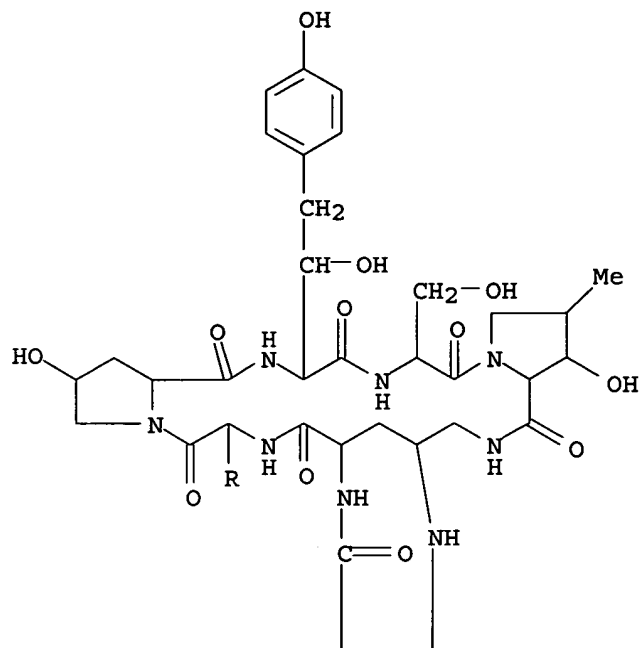
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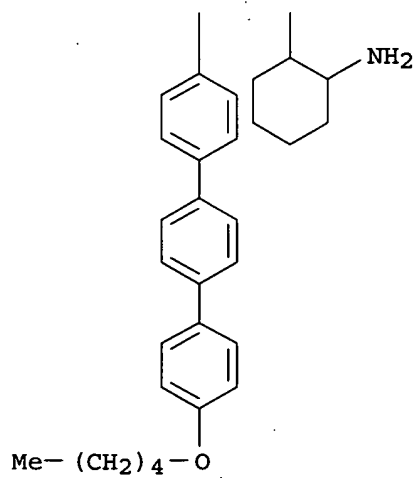
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\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

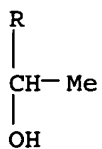
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CN Deoxymulundocandin, 1-[(4S)-4-[(1H-benzimidazol-2-ylmethyl)amino]-N2-[[4'-(pentyloxy)[1,1':4',1''-terphenyl]-4-yl]carbonyl]-L-ornithine]-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)  
 FS PROTEIN SEQUENCE; STEREOSEARCH  
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 LC STN Files: CA, CAPLUS, CASREACT  
 DT.CA Caplus document type: Patent  
 RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

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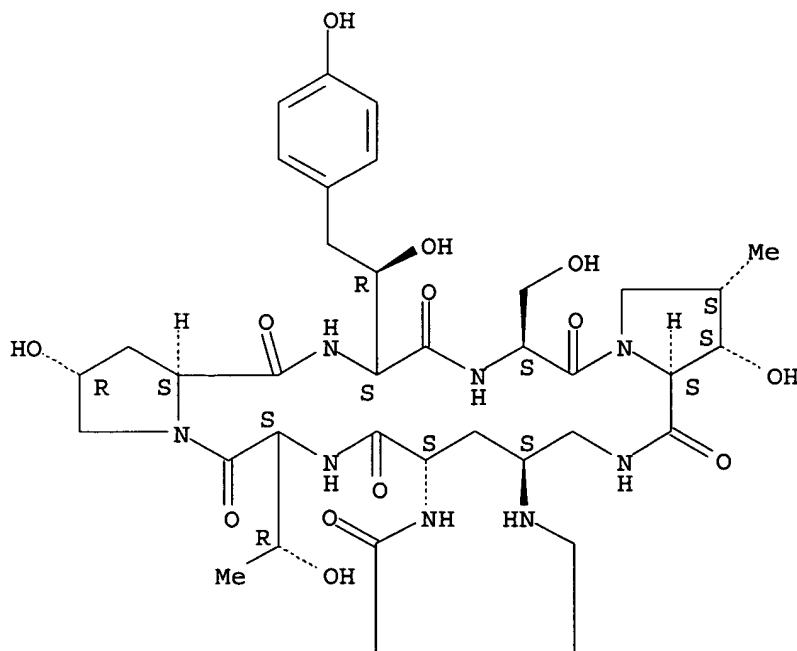
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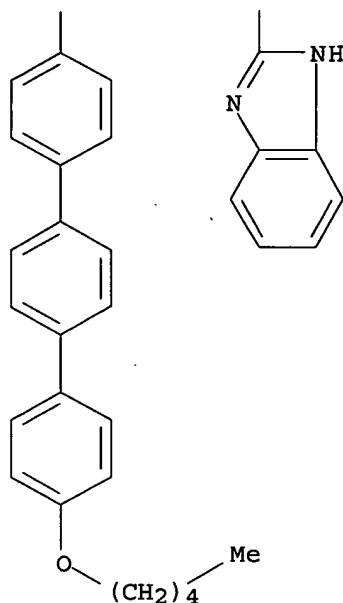
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Absolute stereochemistry.

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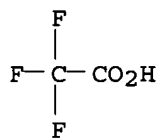
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:17731

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RN 310461-96-2 REGISTRY

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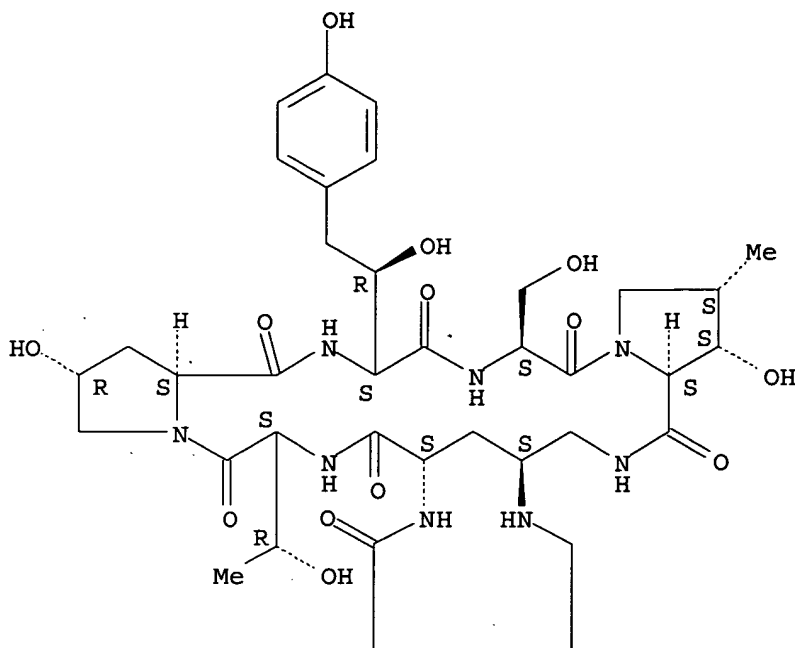
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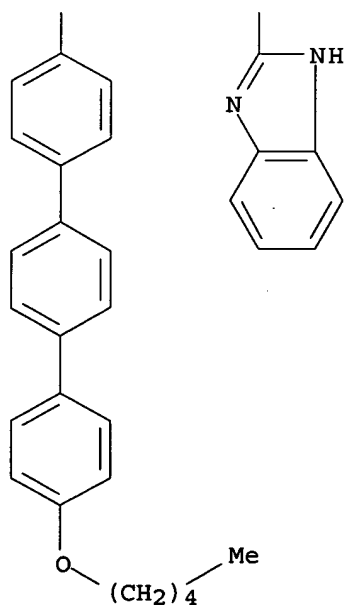
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Absolute stereochemistry.

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SR CA  
LC STN Files: CA, CAPLUS, CASREACT  
DT.CA CAPLUS document type: Patent  
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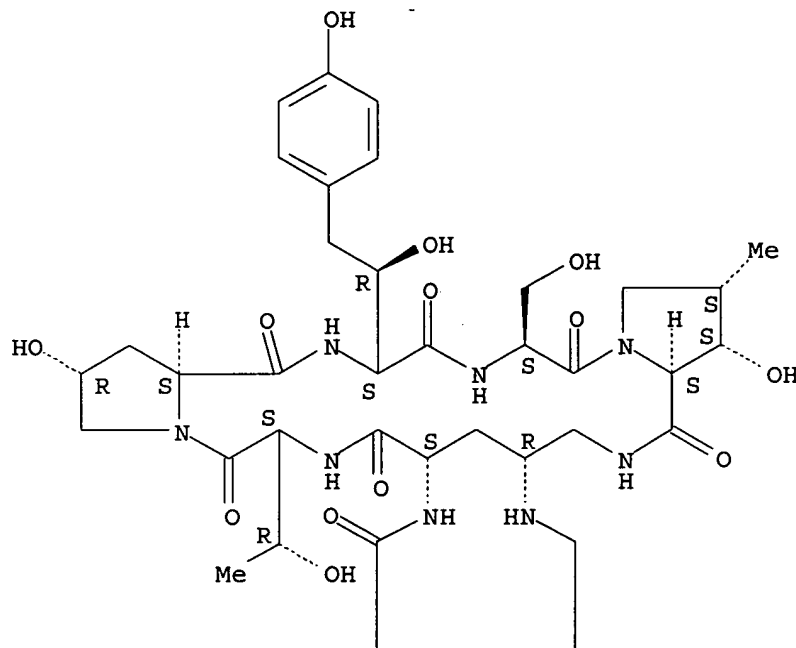
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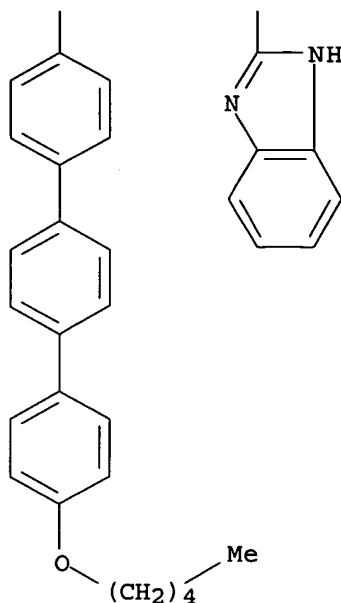
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Absolute stereochemistry.

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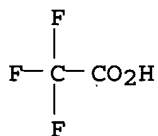
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REFERENCE 1: 134:17731

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RN 310461-94-0 REGISTRY

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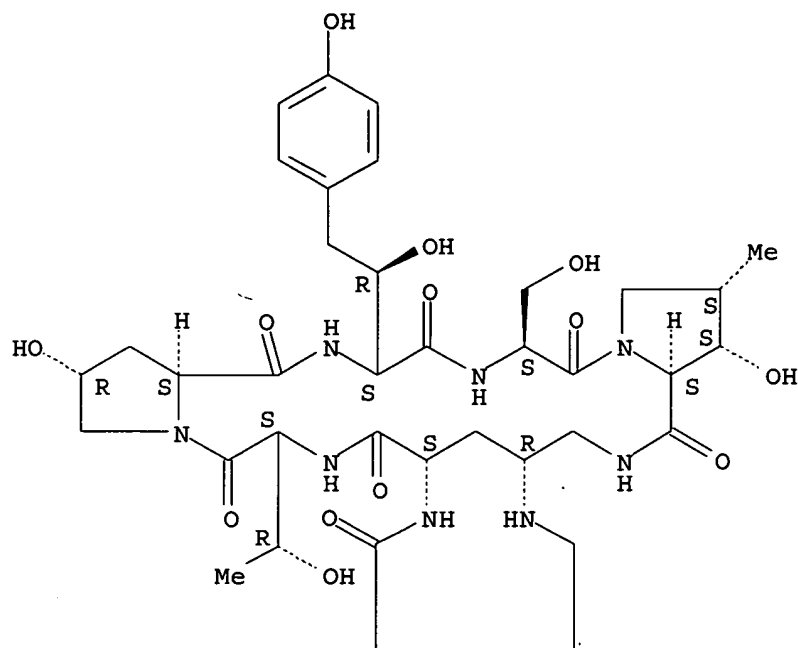
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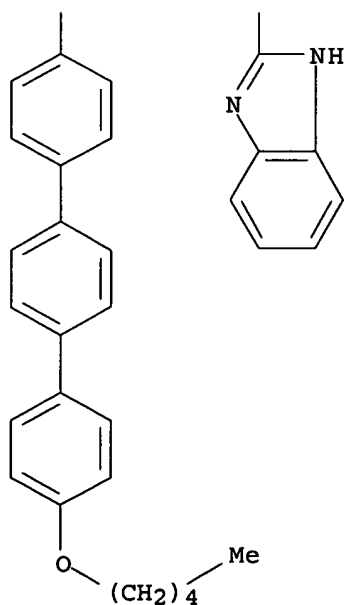
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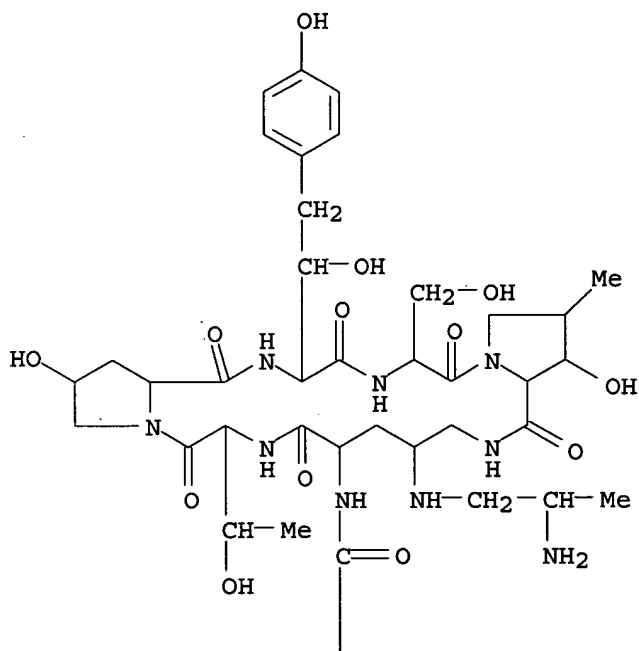
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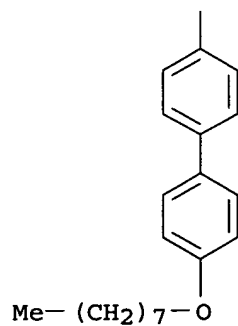
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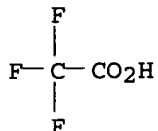


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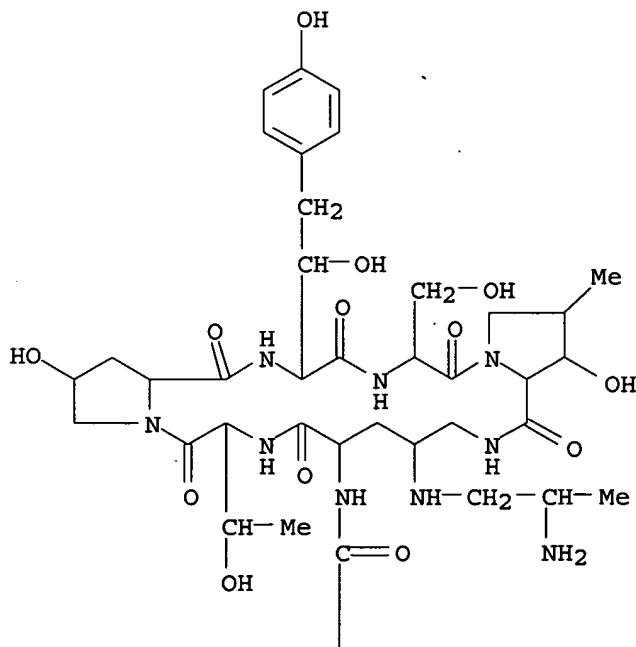
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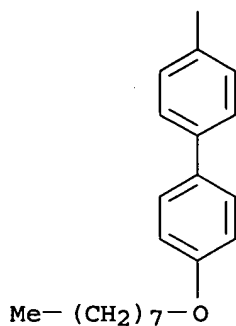
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L3 ANSWER 17 OF 55 REGISTRY COPYRIGHT 2004 ACS on STN  
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MF C57 H81 N9 O14 . x C2 H F3 O2  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT  
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RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

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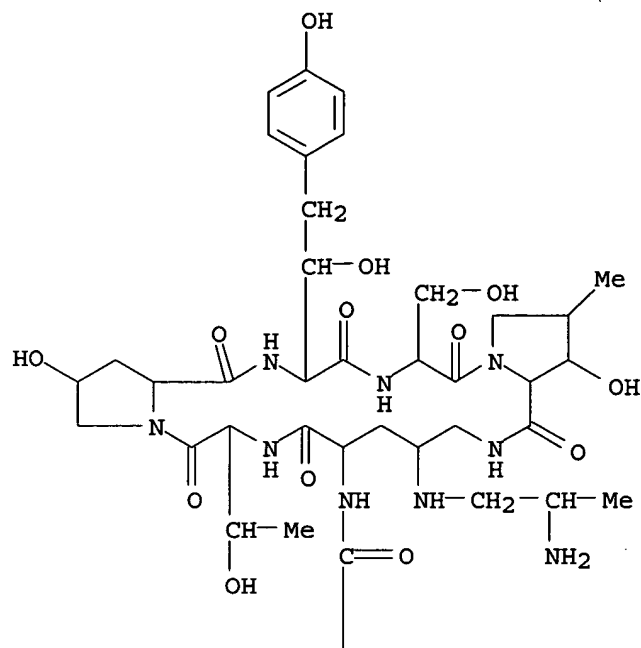
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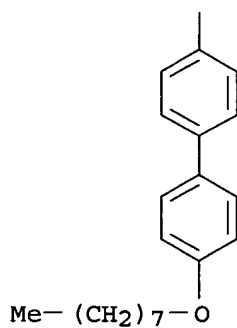
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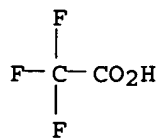
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CRN 76-05-1

CMF C2 H F3 O2



1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:17731

L3 ANSWER 18 OF 55 REGISTRY COPYRIGHT 2004 ACS on STN

RN 310461-85-9 REGISTRY

CN Deoxymulundocandin, 1-[(4R)-4-[[[(2S)-2-aminopropyl]amino]-N2-[[4'-(octyloxy)[1,1'-biphenyl]-4-yl]carbonyl]-L-ornithine]- (9CI) (CA INDEX NAME)

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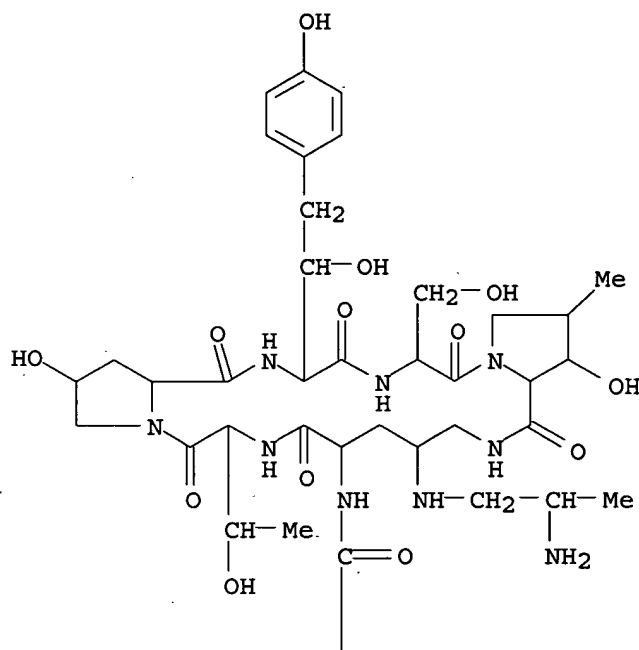
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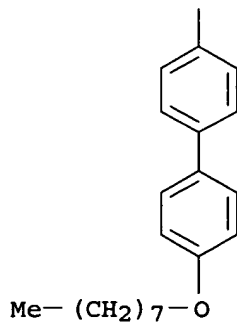
SR CA

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

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L3 ANSWER 19 OF 55 REGISTRY COPYRIGHT 2004 ACS on STN

RN 310459-70-2 REGISTRY



CN Deoxymulundocandin, 1-[(4S)-4-[[[(1R,2R)-2-aminocyclohexyl]amino]-N2-[4-[5-[4-(pentyloxy)phenyl]-1,3,4-thiadiazol-2-yl]benzoyl]-L-ornithine]-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C59 H79 N11 O14 S . x C2 H F3 O2  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT  
DT.CA Caplus document type: Patent  
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

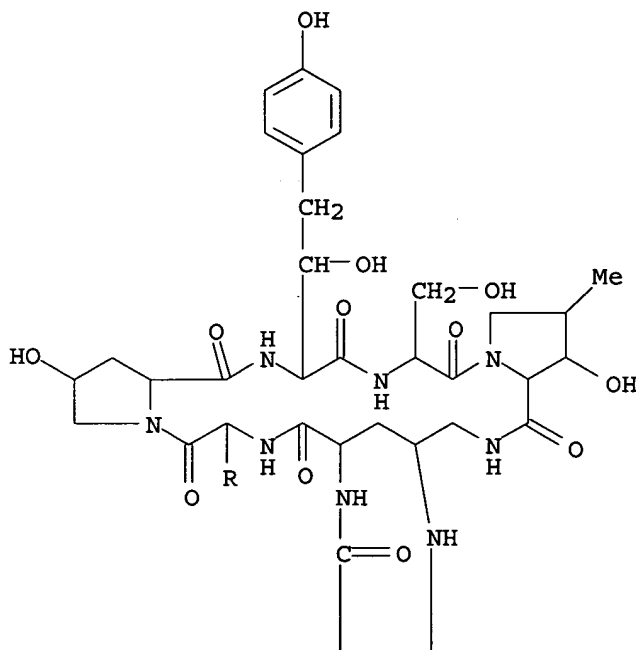
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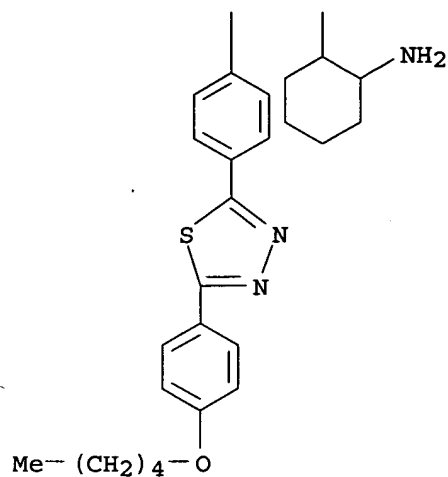
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\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

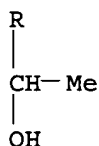
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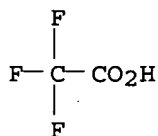
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CM 2

CRN 76-05-1

CMF C2 H F3 O2



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:17732

L3 ANSWER 20 OF 55 REGISTRY COPYRIGHT 2004 ACS on STN

RN 310459-69-9 REGISTRY

CN Deoxymulundocandin, 1-[(4S)-4-[[[(1R,2R)-2-aminocyclohexyl]amino]-N2-[4-[5-[4-(pentyloxy)phenyl]-1,3,4-thiadiazol-2-yl]benzoyl]-L-ornithine]- (9CI)  
(CA INDEX NAME)

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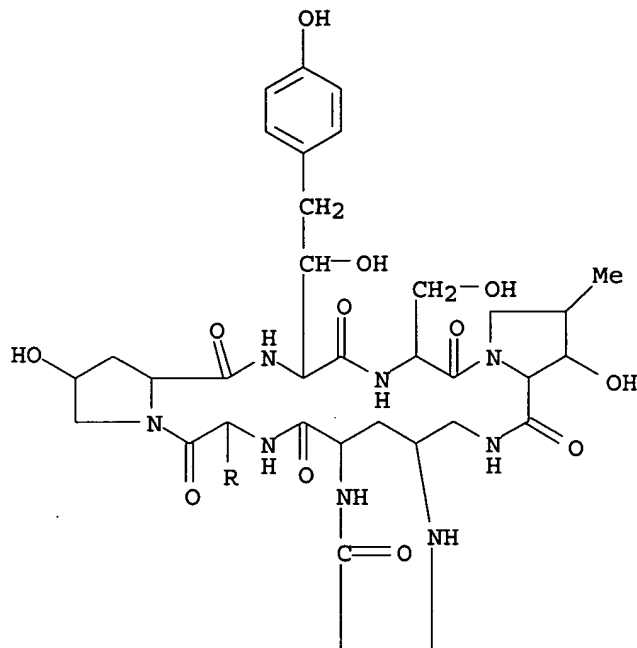
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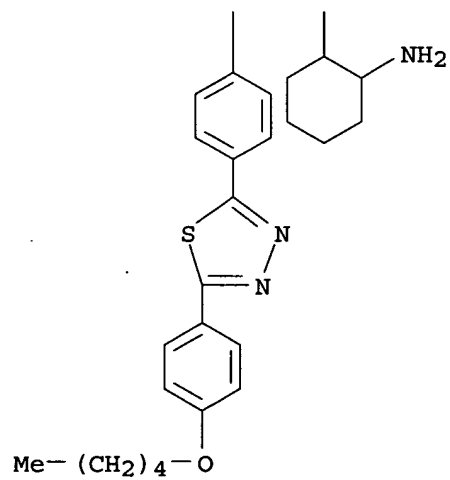
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\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

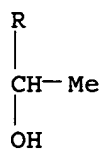
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CN Deoxymulundocandin, 1-[(4R)-4-[[[(1R,2R)-2-aminocyclohexyl]amino]-N2-[4-[5-[4-(pentyloxy)phenyl]-1,3,4-thiadiazol-2-yl]benzoyl]-L-ornithine]-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)  
 FS PROTEIN SEQUENCE; STEREOSEARCH  
 MF C59 H79 N11 O14 S . x C2 H F3 O2  
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 LC STN Files: CA, CAPLUS, CASREACT  
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 RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

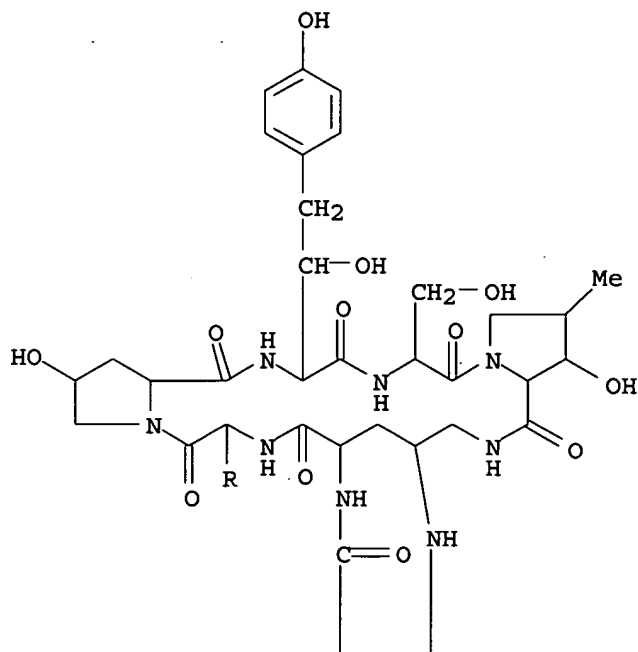
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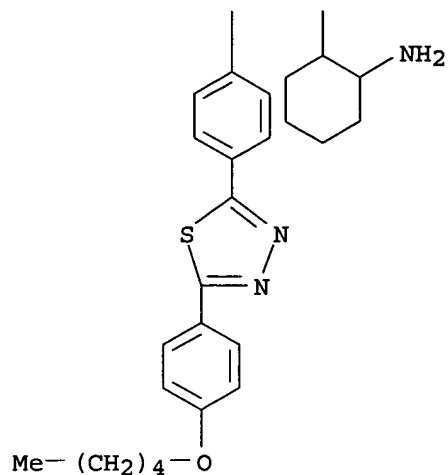
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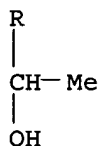
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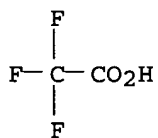
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CRN 76-05-1

CMF C2 H F3 O2



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:17732

L3 ANSWER 22 OF 55 REGISTRY COPYRIGHT 2004 ACS on STN

RN 310459-66-6 REGISTRY

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(CA INDEX NAME)

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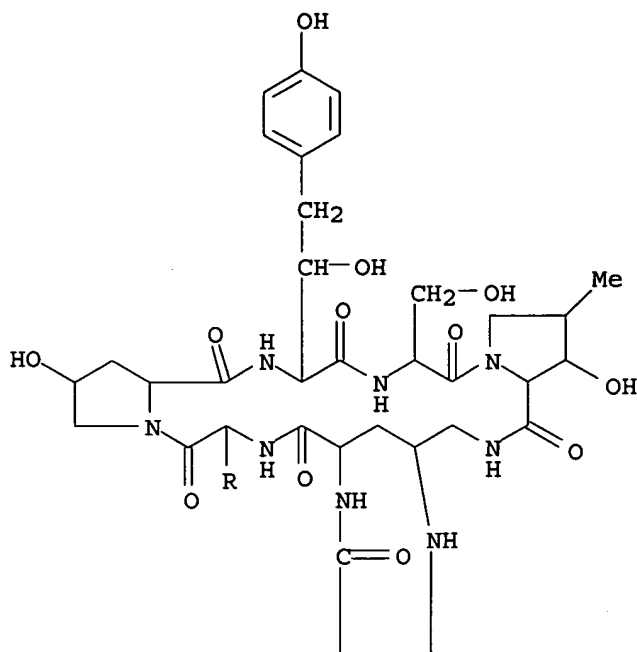
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CI COM

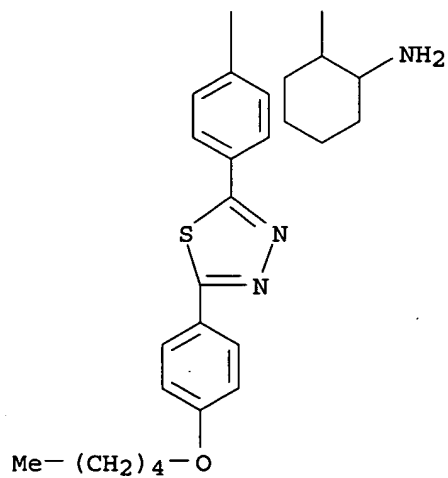
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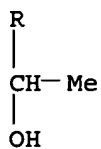
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CN Deoxymulundocandin, 1-[(4S)-4-[[[(1S,2S)-2-aminocyclohexyl]amino]-N2-[4-[5-[4-(pentyloxy)phenyl]-1,3,4-thiadiazol-2-yl]benzoyl]-L-ornithine]-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)  
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SR CA  
LC STN Files: CA, CAPLUS, CASREACT  
DT.CA Caplus document type: Patent  
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

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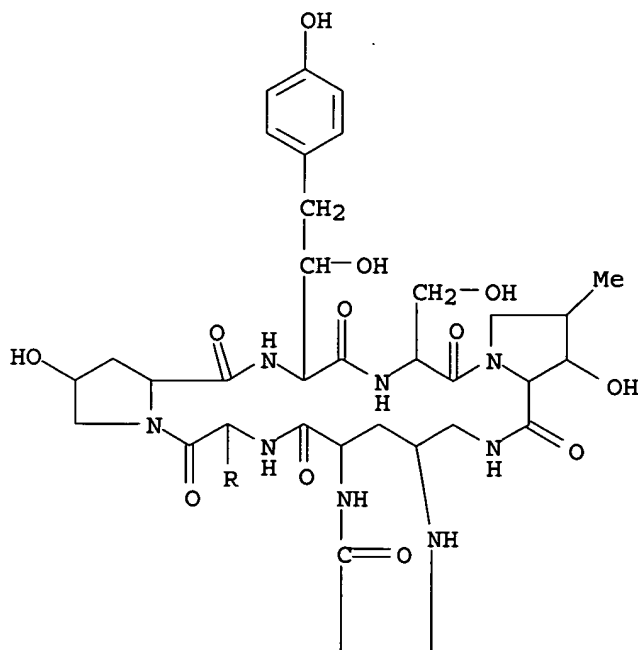
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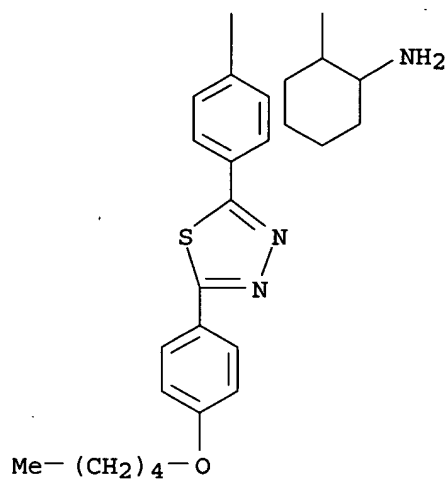
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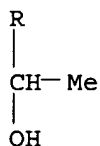
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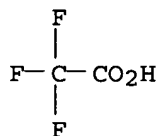
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1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:17732

L3 ANSWER 24 OF 55 REGISTRY COPYRIGHT 2004 ACS on STN

RN 310459-60-0 REGISTRY

CN Deoxymulundocandin, 1-[[[(1S,2S)-2-aminocyclohexyl]amino]-N2-[4-[5-[4-(pentyloxy)phenyl]-1,3,4-thiadiazol-2-yl]benzoyl]-L-ornithine]- (9CI)  
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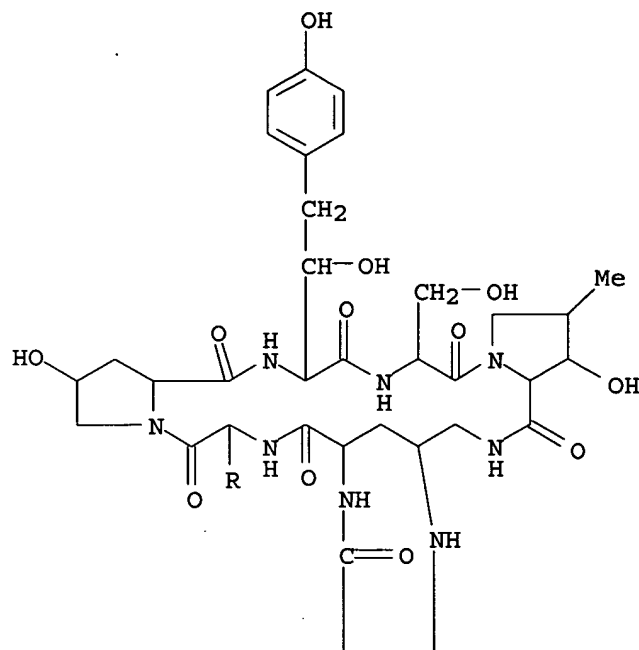
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SR CA

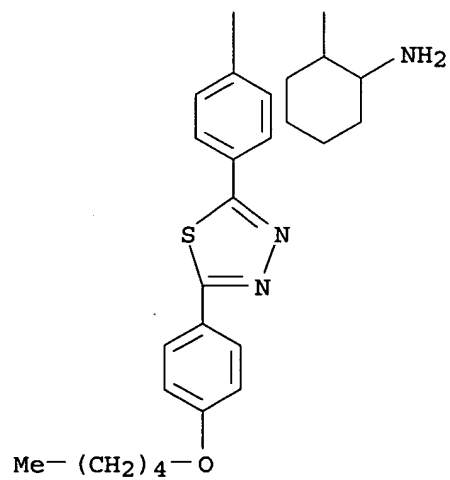
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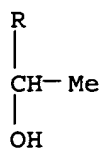
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CN Deoxymulundocandin, 1-[(4R)-4-[[[(1S,2S)-2-aminocyclohexyl]amino]-N2-[4-[5-[4-(pentyloxy)phenyl]-1,3,4-thiadiazol-2-yl]benzoyl]-L-ornithine]-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C59 H79 N11 O14 S . x C2 H F3 O2  
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LC STN Files: CA, CAPLUS, CASREACT  
DT.CA Caplus document type: Patent  
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

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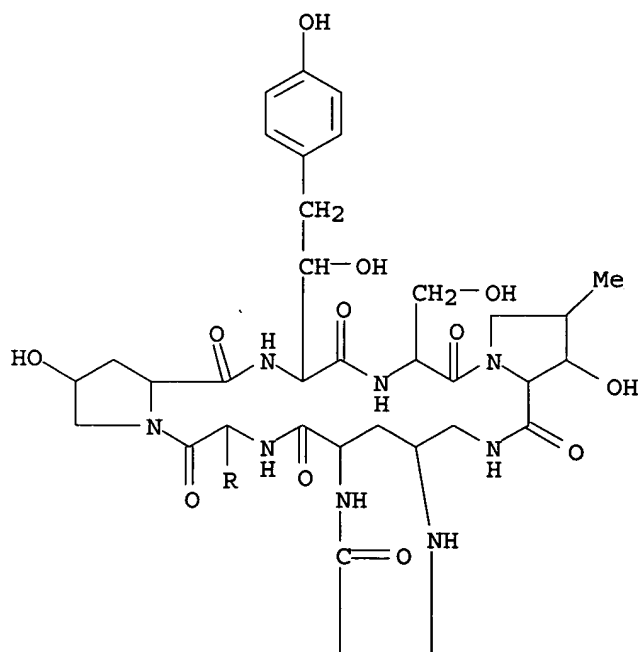
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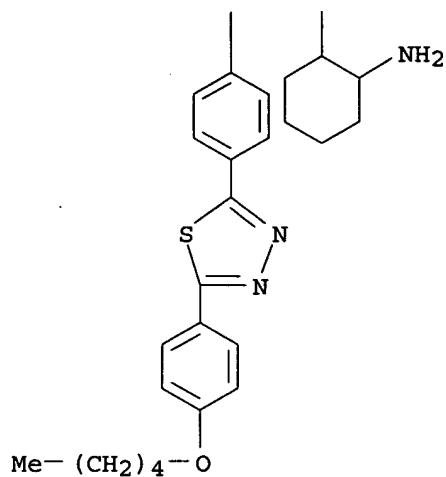
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\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

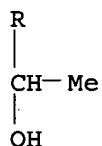
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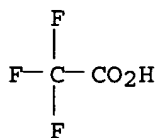
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PAGE 3-A



CM 2  
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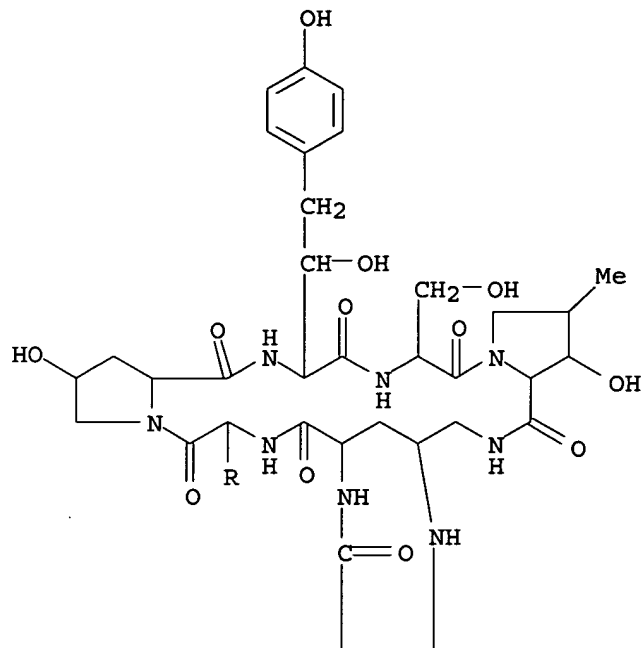
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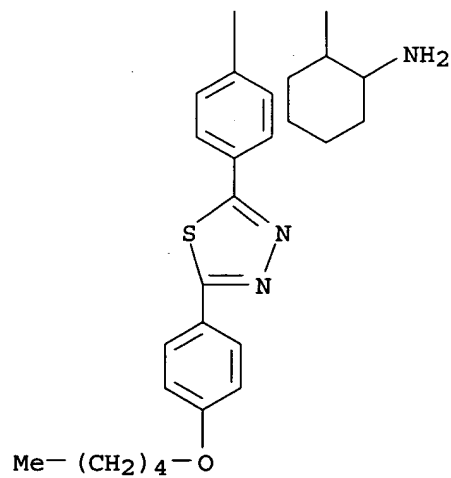
L3 ANSWER 26 OF 55 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 310459-57-5 REGISTRY  
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(CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C59 H79 N11 O14 S  
CI COM  
SR CA

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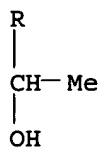
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CN Deoxymulundocandin, 1-[(4S)-4-[(2-aminoethyl)amino]-N2-[4-[5-[4-(pentyloxy)phenyl]-1,3,4-thiadiazol-2-yl]benzoyl]-L-ornithine]-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)  
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LC STN Files: CA, CAPLUS, CASREACT  
DT.CA Caplus document type: Patent  
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

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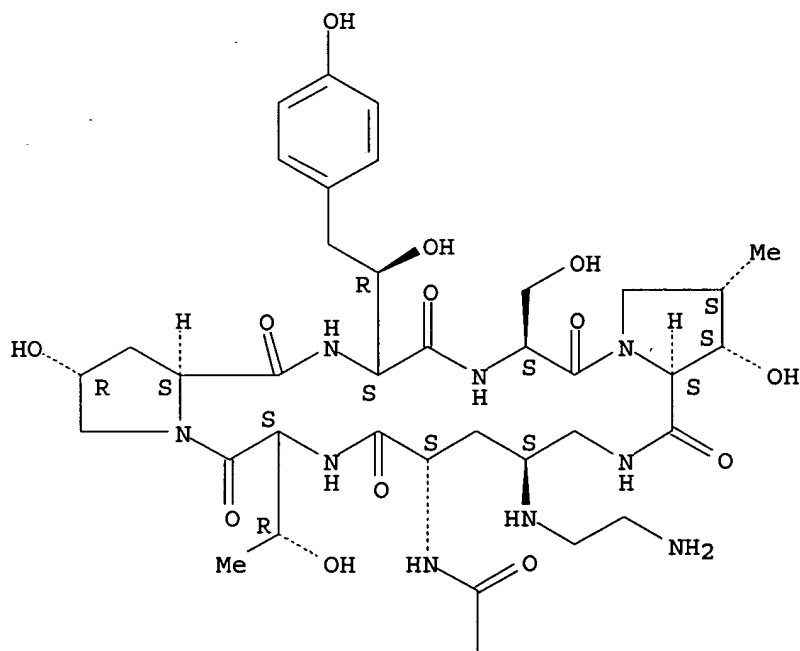
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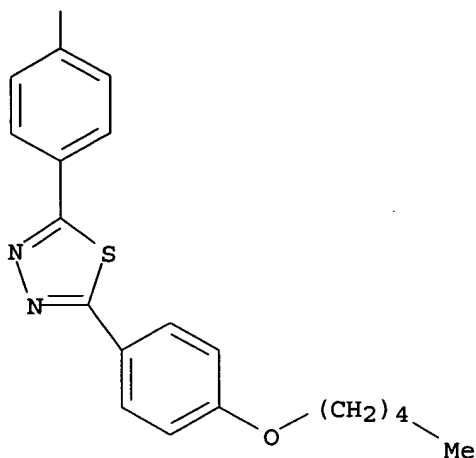
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Absolute stereochemistry.

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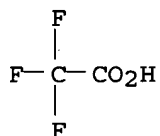
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CM 2

CRN 76-05-1

CMF C2 H F3 O2



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:17732

L3 ANSWER 28 OF 55 REGISTRY COPYRIGHT 2004 ACS on STN

RN 310459-51-9 REGISTRY

CN Deoxymulundocandin, 1-[(4S)-4-[(2-aminoethyl)amino]-N2-[4-[5-[4-(pentyloxy)phenyl]-1,3,4-thiadiazol-2-yl]benzoyl]-L-ornithine]- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C55 H73 N11 O14 S

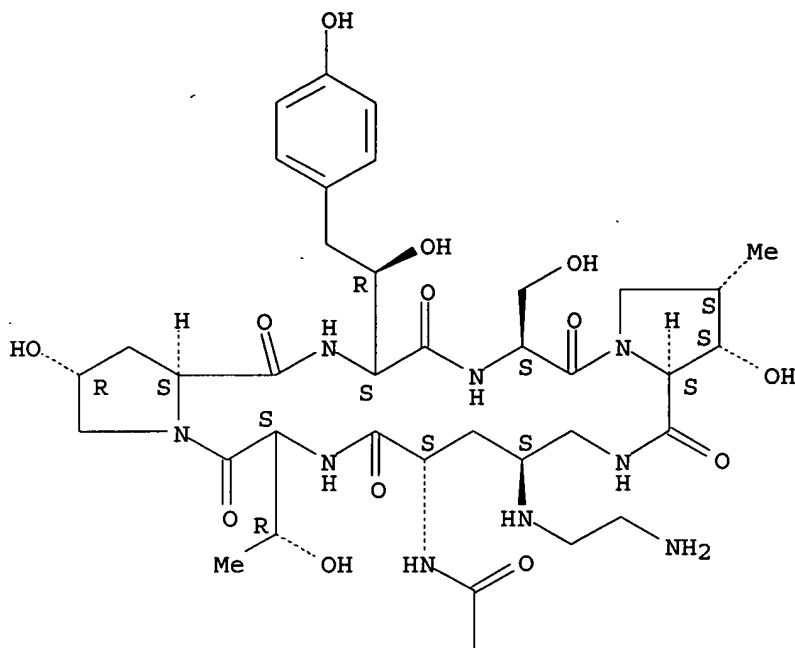
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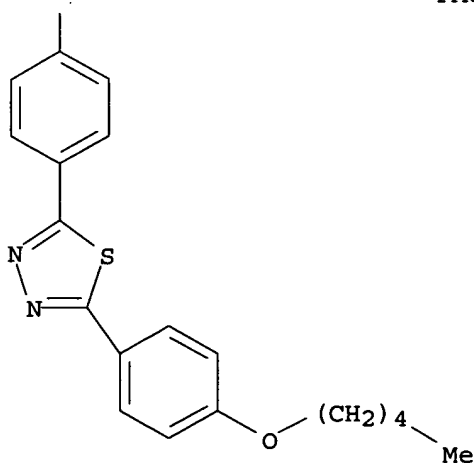
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 FS PROTEIN SEQUENCE; STEREOSEARCH  
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 LC STN Files: CA, CAPLUS, CASREACT  
 DT.CA Caplus document type: Patent  
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**\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\***

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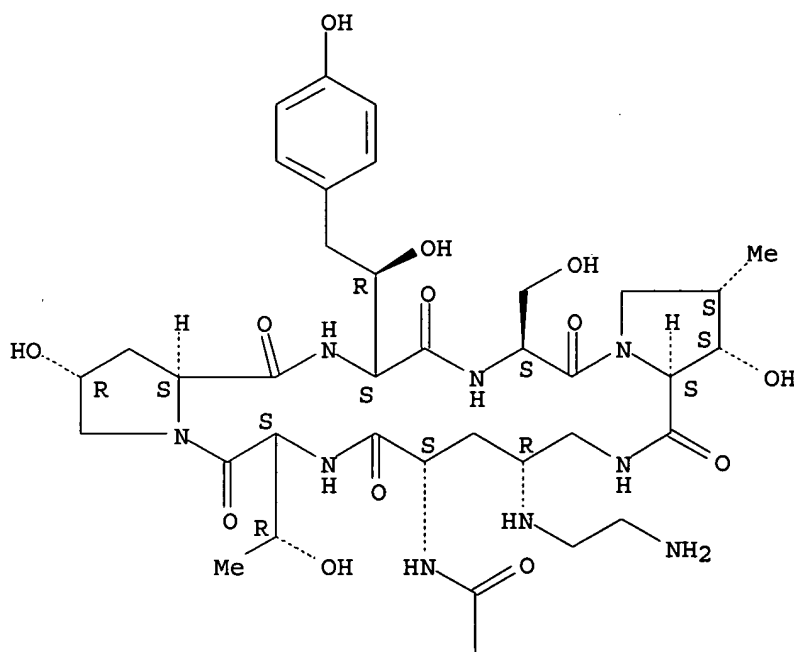
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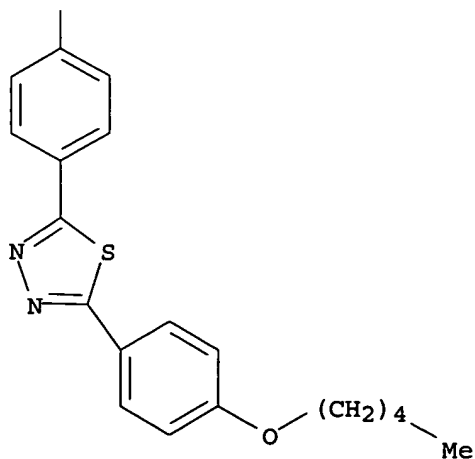
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Absolute stereochemistry.

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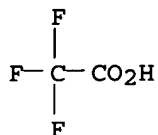
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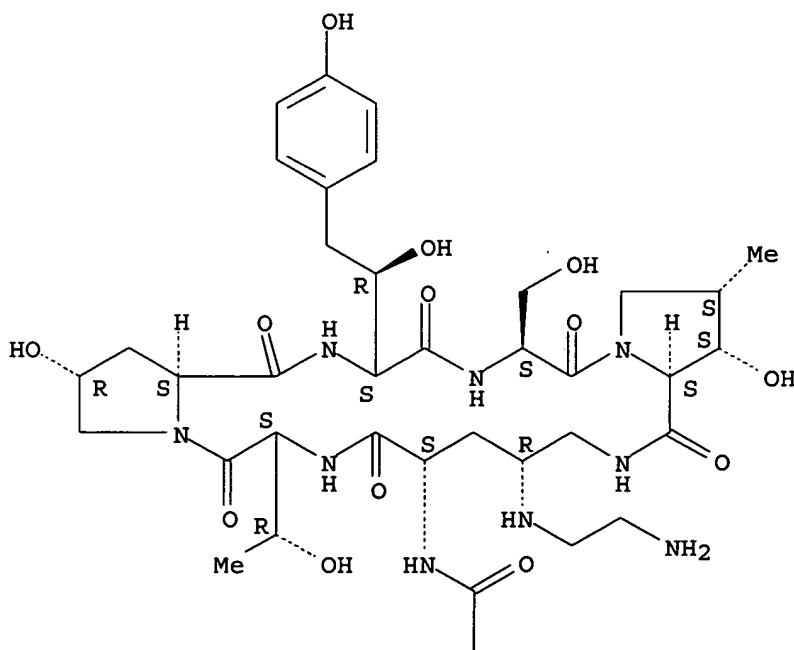
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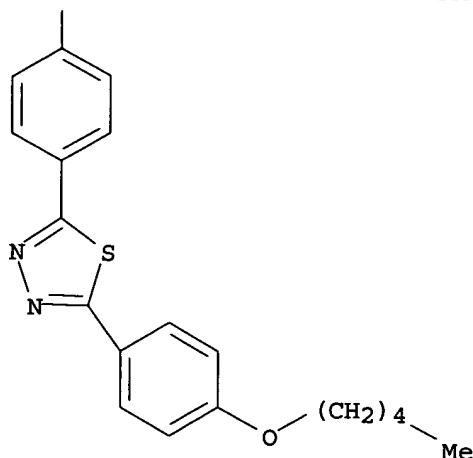
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Absolute stereochemistry.

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:53314

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RN 310459-42-8 REGISTRY  
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FS PROTEIN SEQUENCE; STEREOSEARCH  
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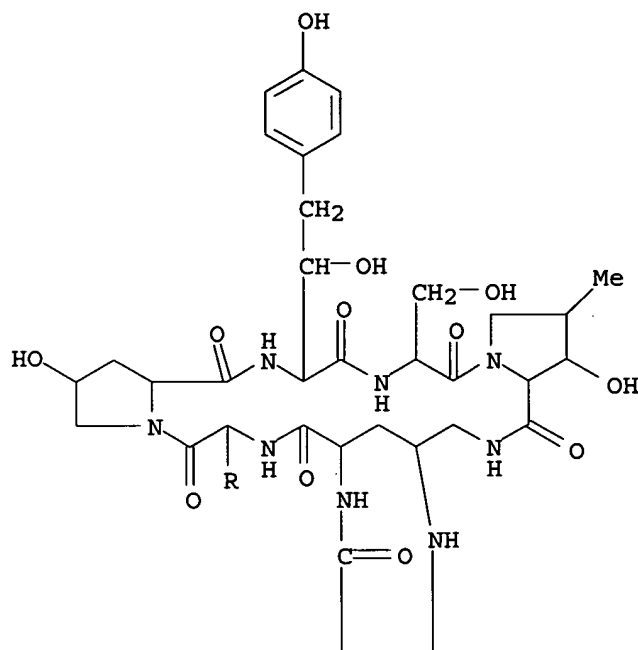
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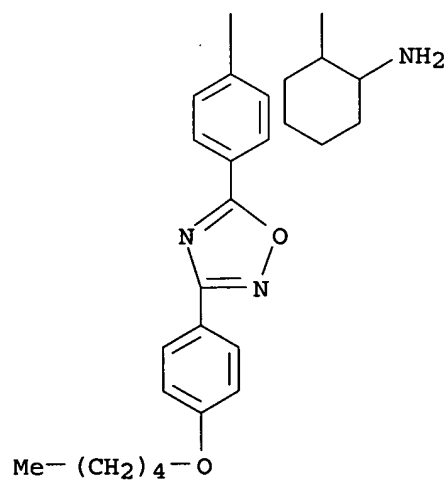
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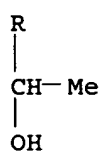
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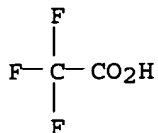
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CRN 76-05-1  
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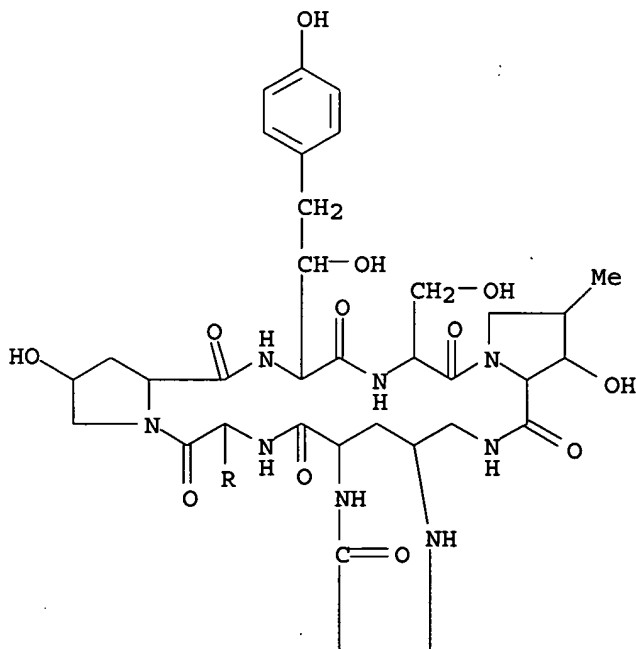
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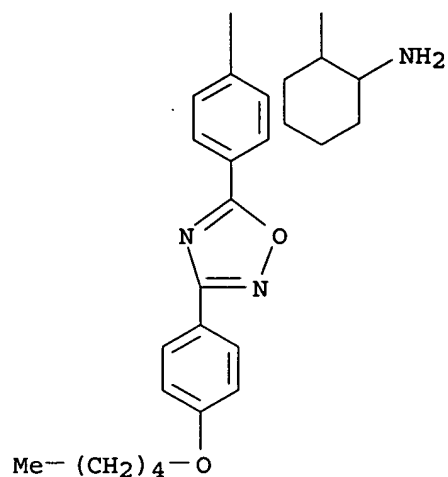
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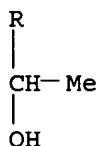
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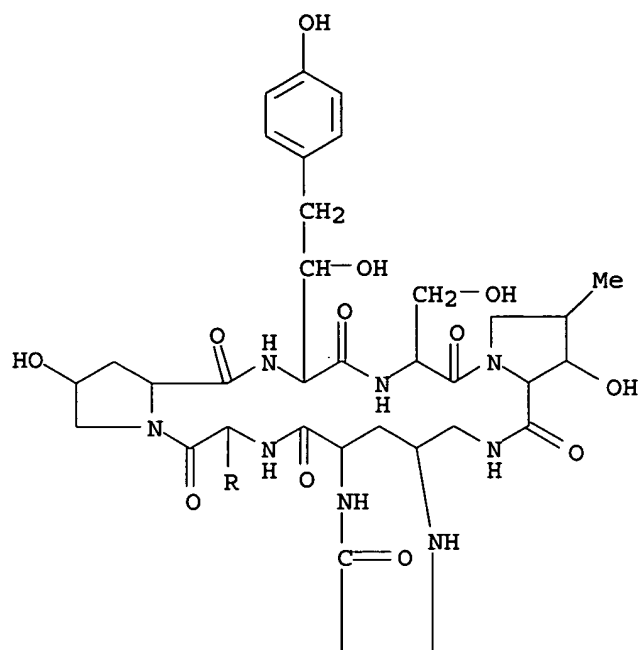
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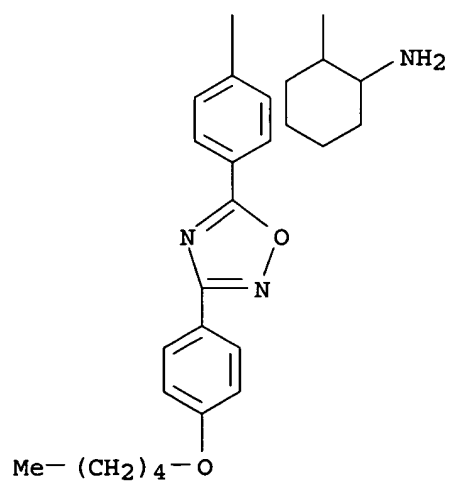
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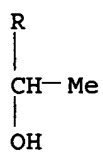
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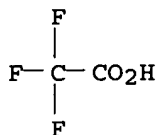
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CRN 76-05-1  
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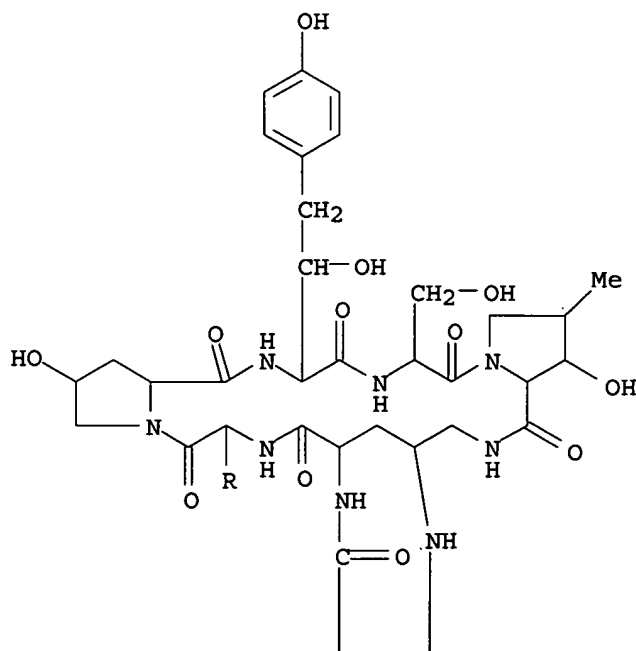
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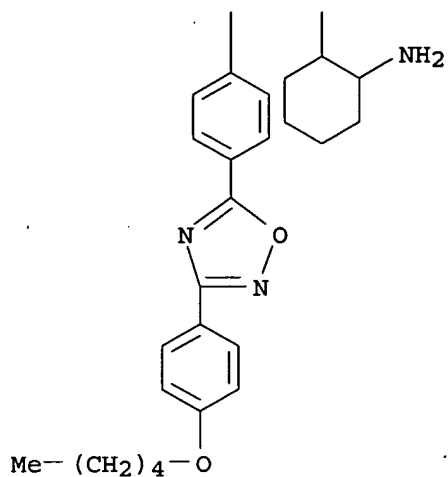
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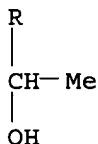
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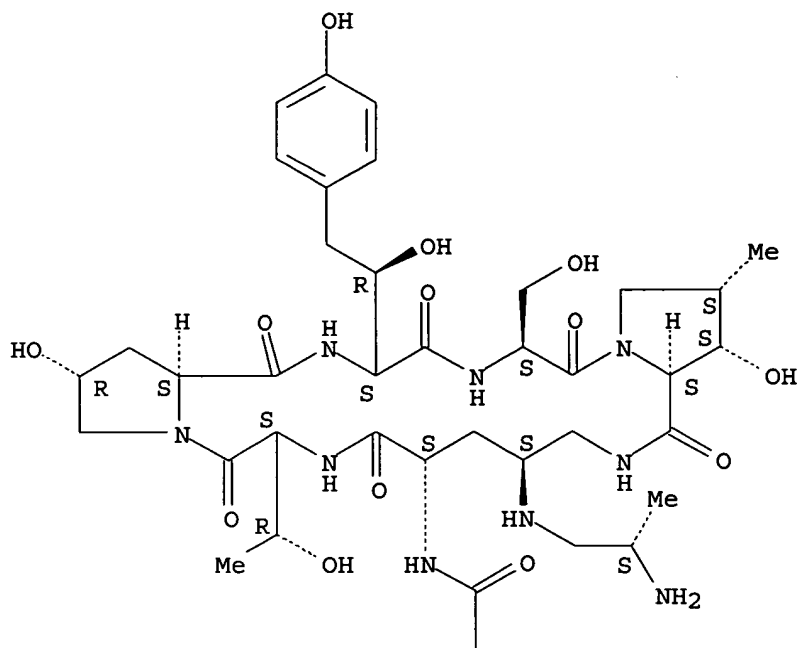
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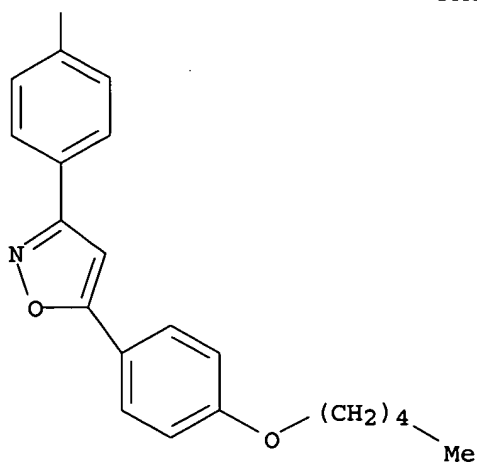
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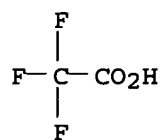
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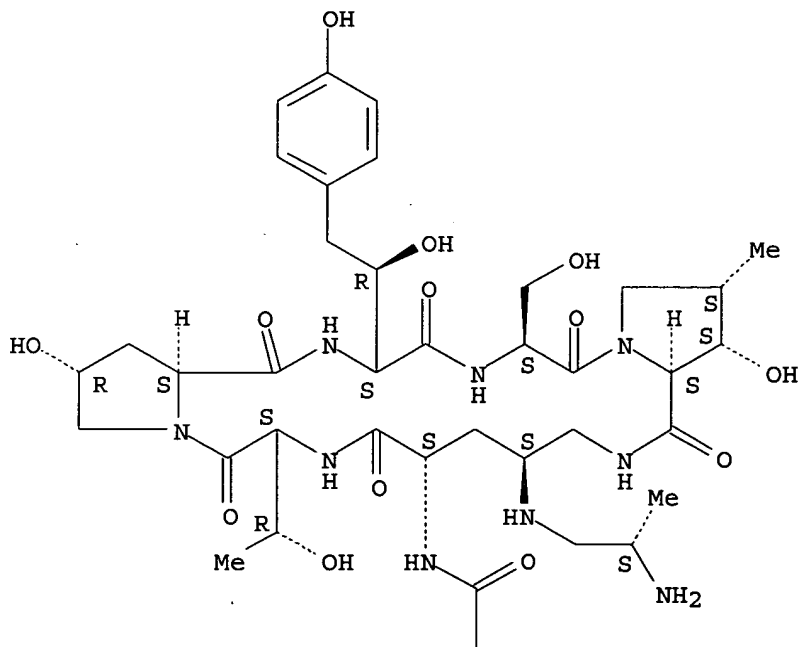
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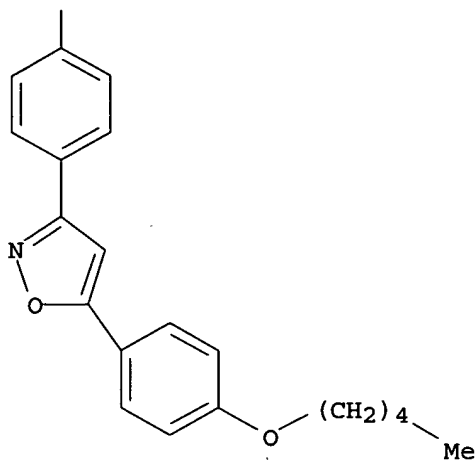
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Absolute stereochemistry.

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SR CA  
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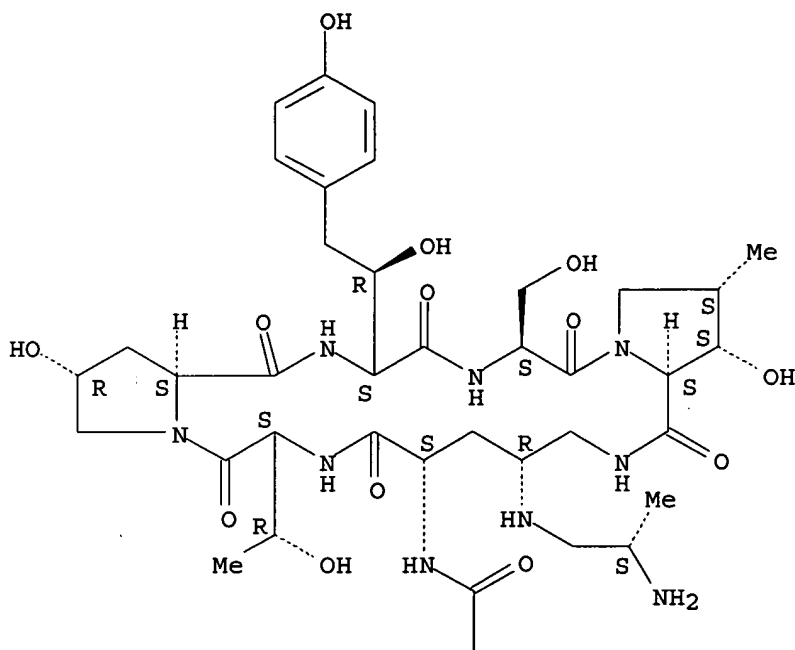
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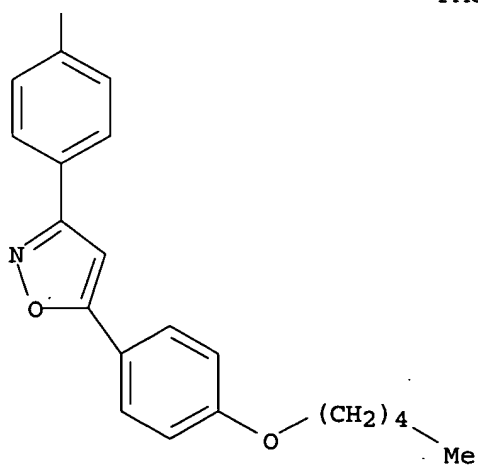
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Absolute stereochemistry.

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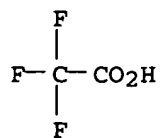
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CRN 76-05-1

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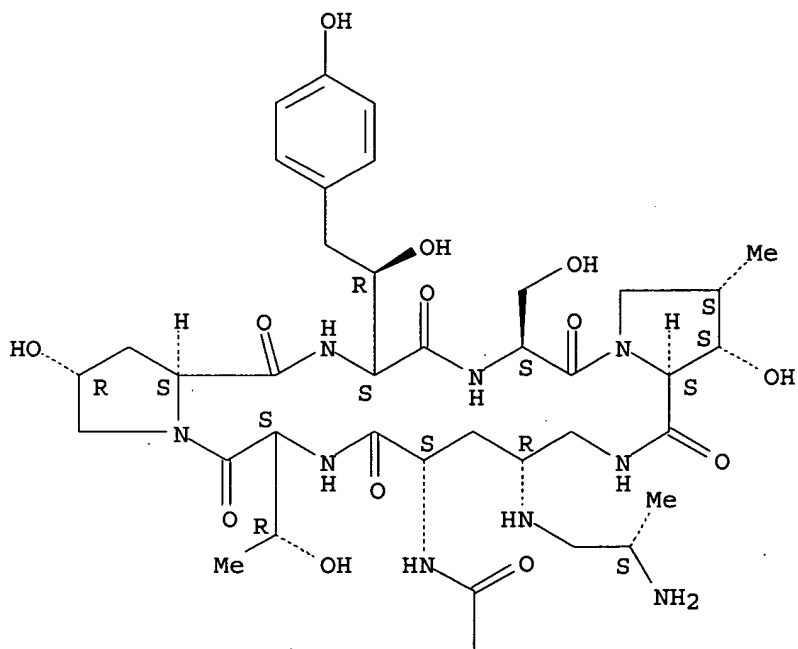
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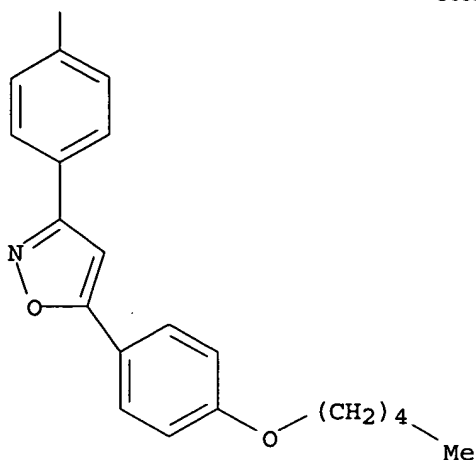
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Absolute stereochemistry.

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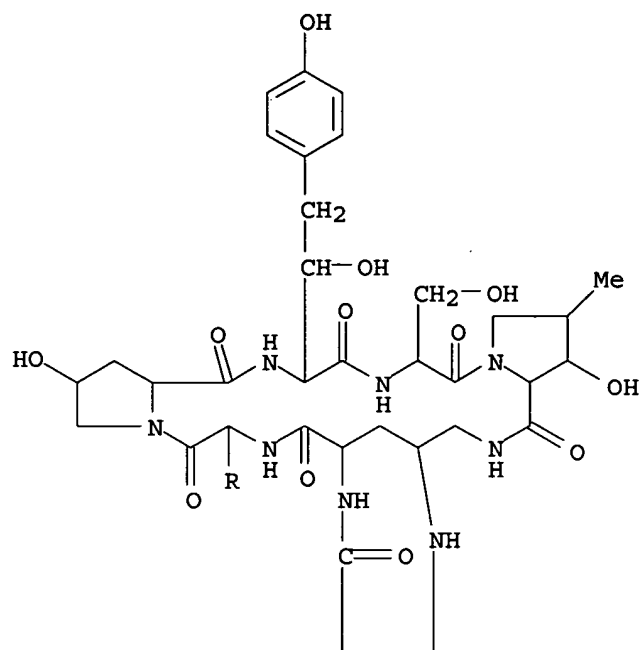
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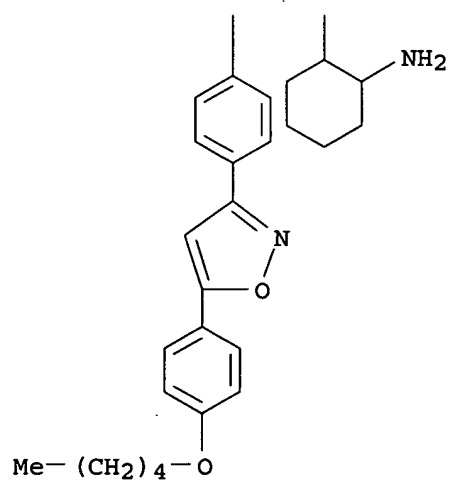
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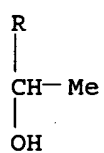
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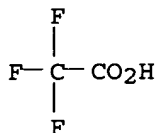
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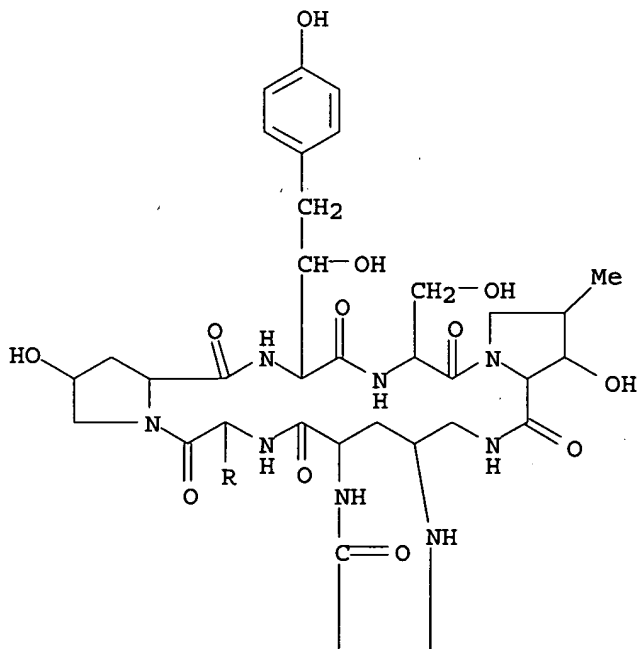
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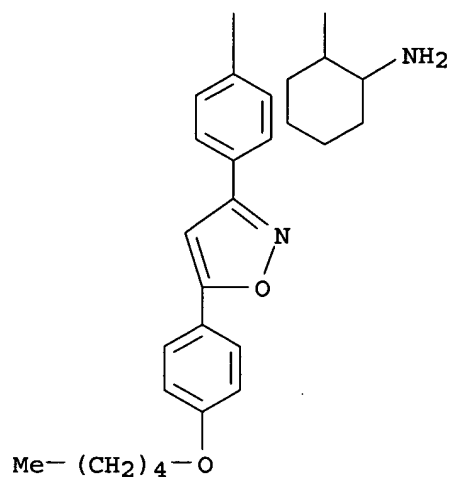
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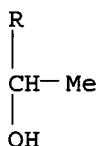




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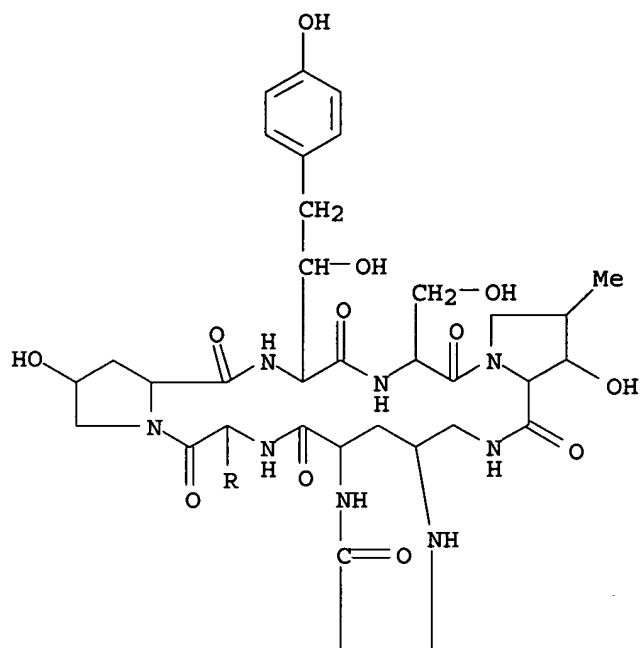
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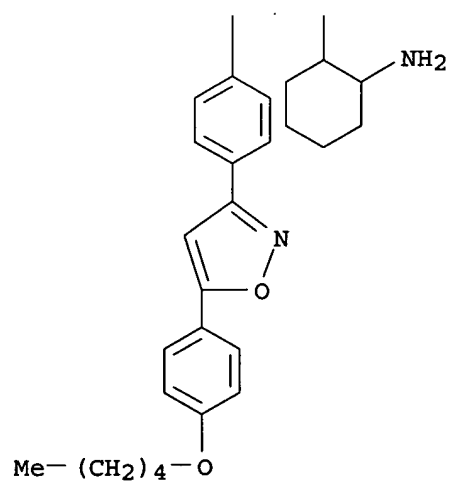
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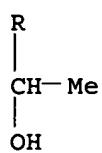
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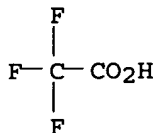
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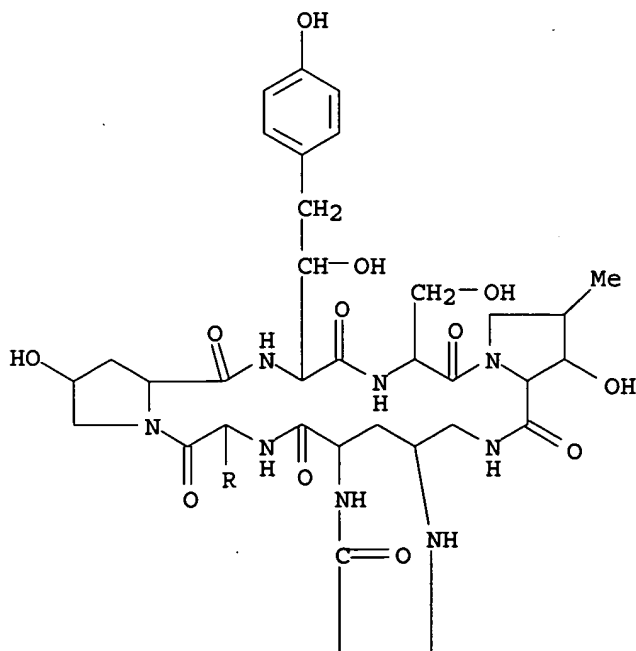
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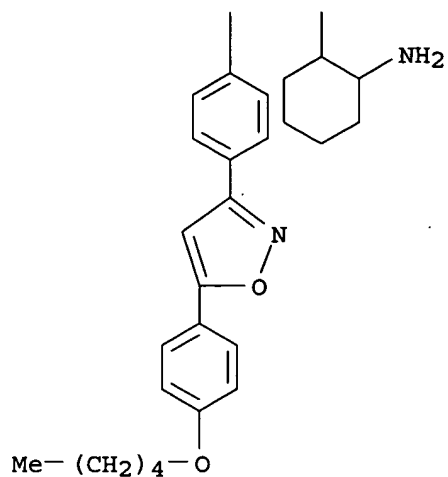
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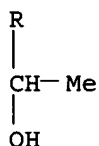
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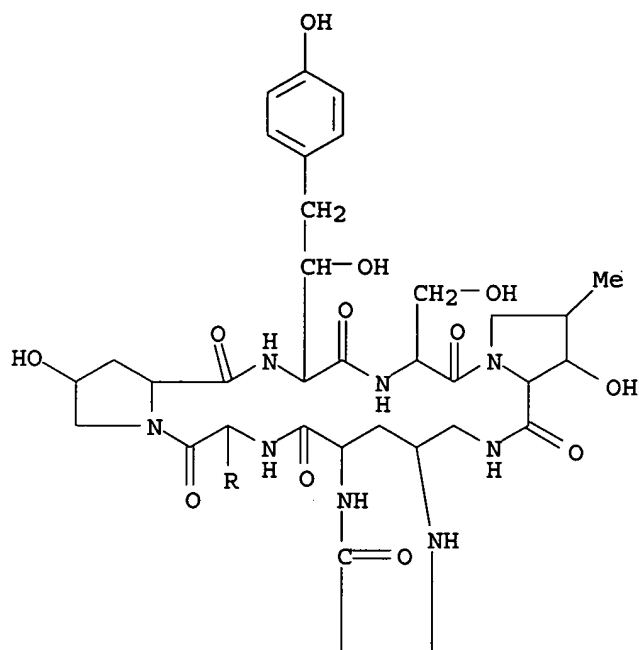
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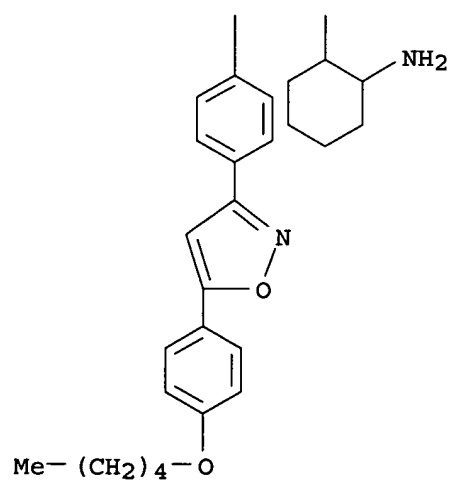
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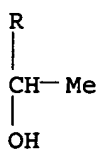
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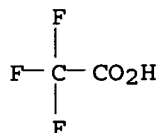
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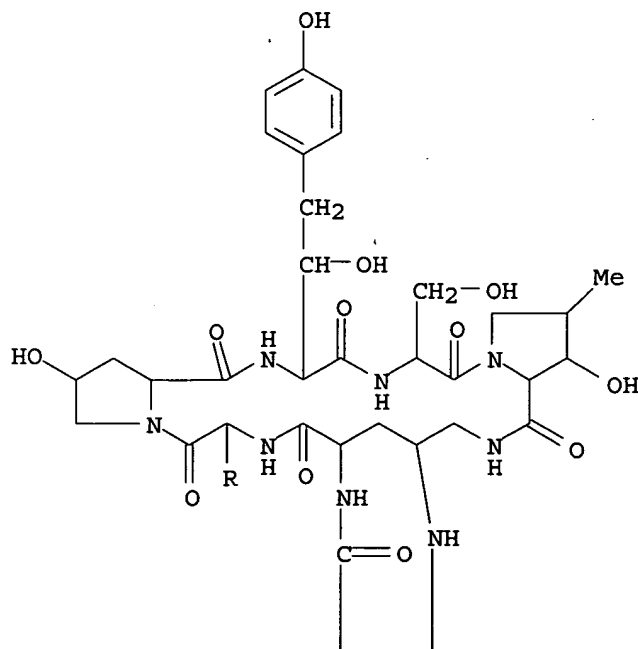
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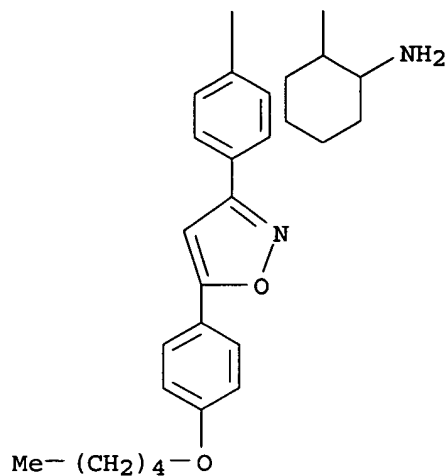
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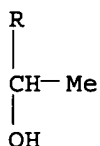
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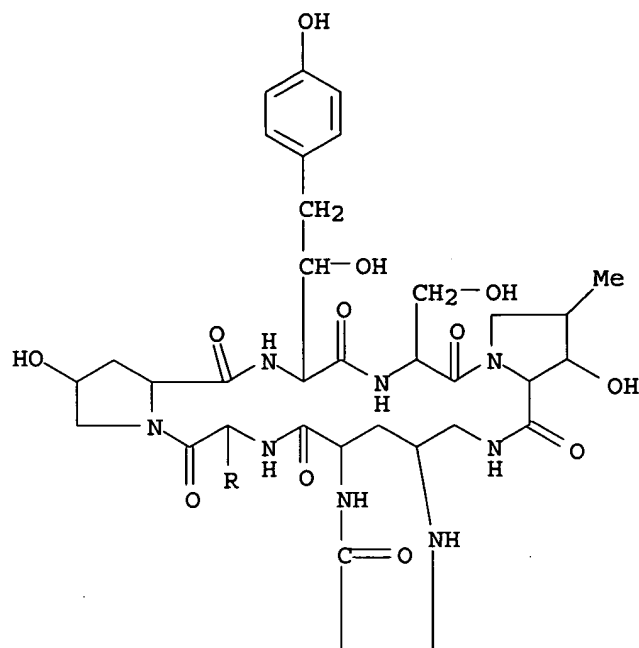
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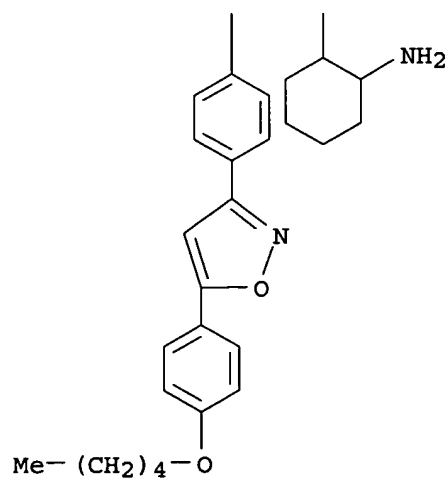
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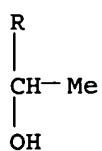
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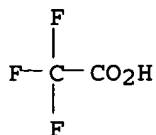


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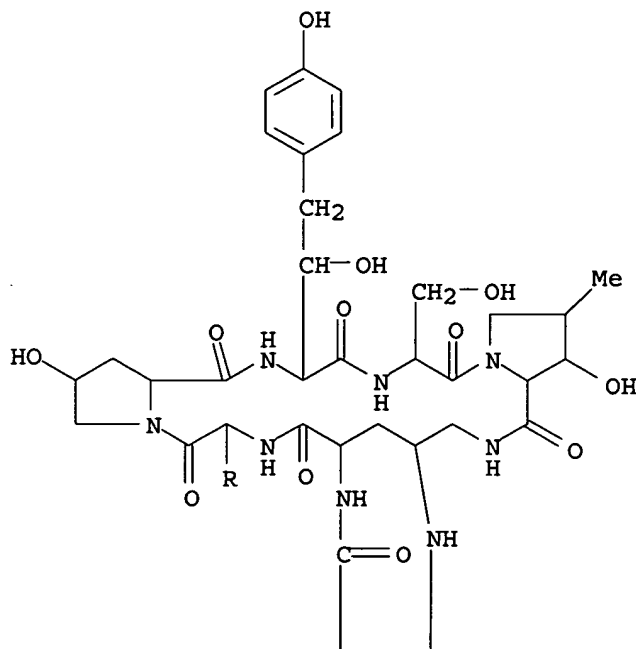
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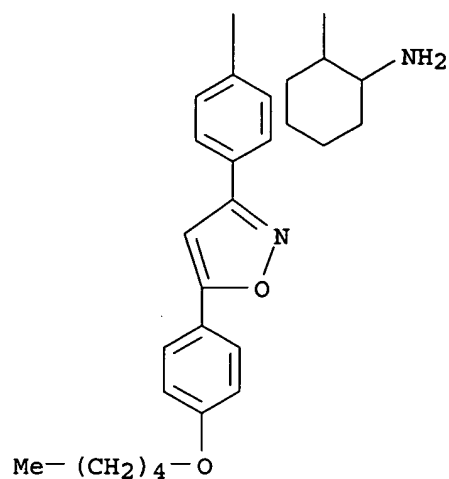
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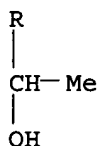
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 RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

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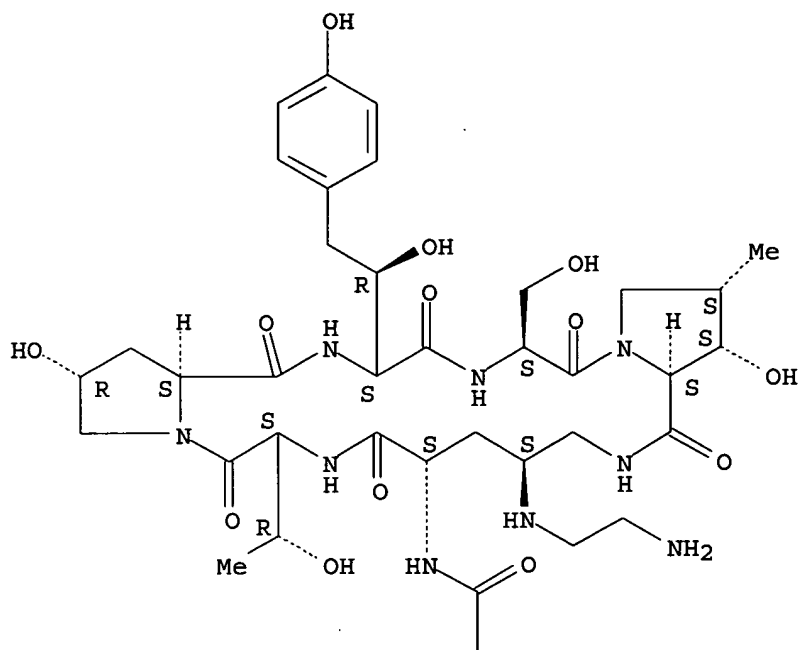
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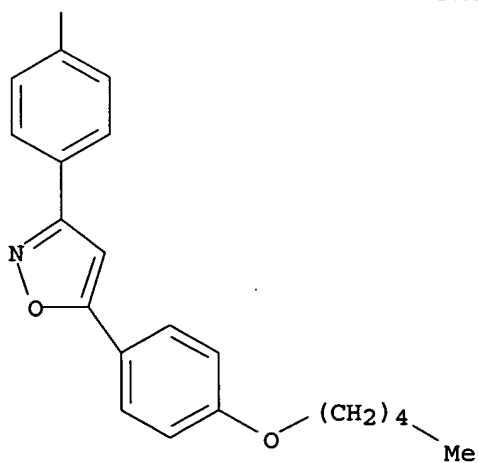
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Absolute stereochemistry.

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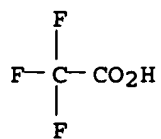


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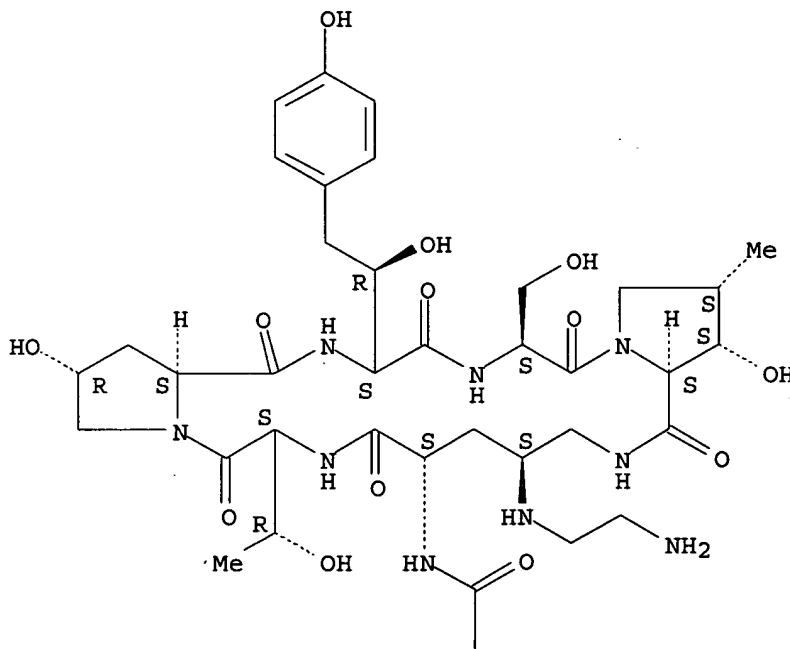
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SR CA

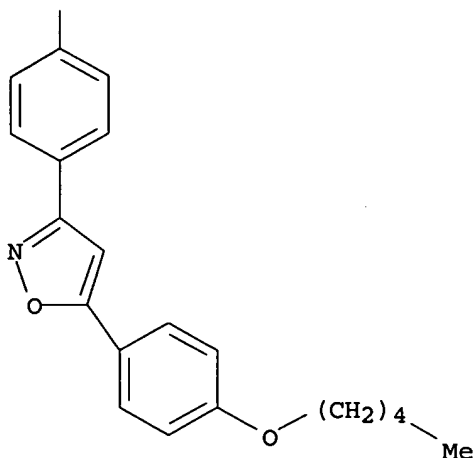
\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.

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L3 ANSWER 49 OF 55 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 310459-08-6 REGISTRY  
CN Deoxymulundocandin, 1-[(4R)-4-[(2-aminoethyl)amino]-N2-[4-[5-[4-(pentyloxy)phenyl]-3-isoxazolyl]benzoyl]-L-ornithine]-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C56 H74 N10 O15 . x C2 H F3 O2  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT  
DT.CA Caplus document type: Patent  
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

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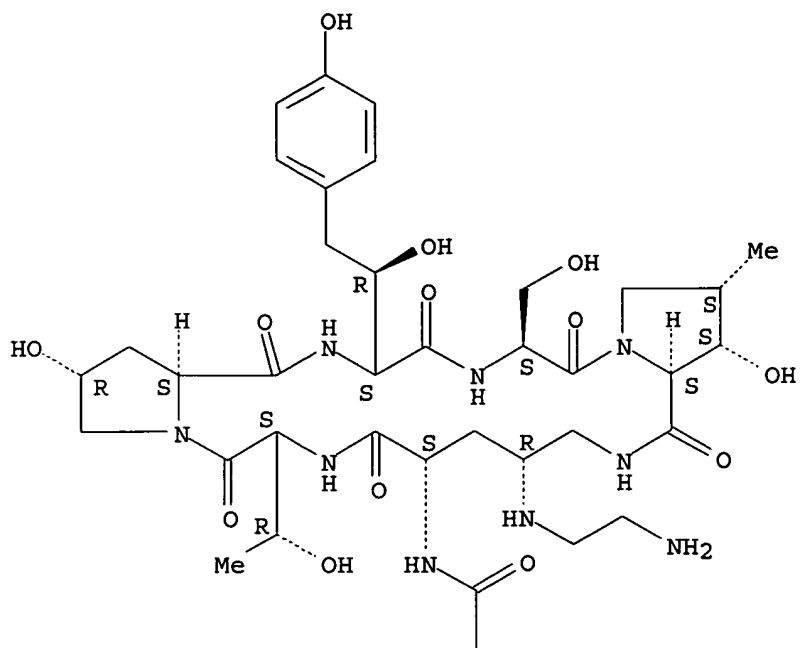
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CMF C56 H74 N10 O15

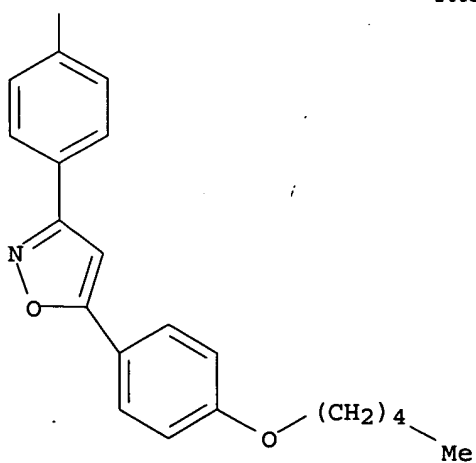
\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.

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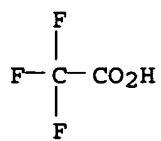


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CM 2

CRN 76-05-1  
CMF C2 H F3 O2



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

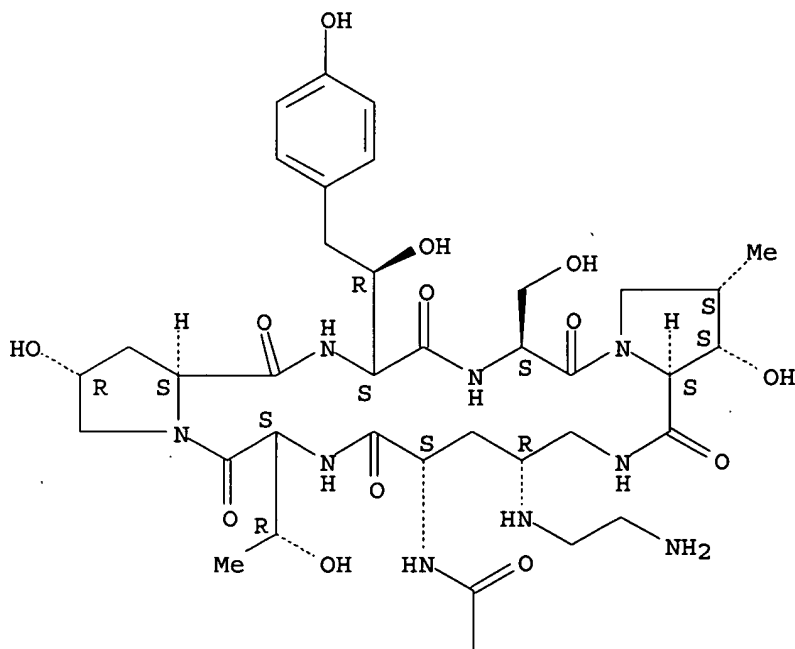
REFERENCE 1: 134:17732

L3 ANSWER 50 OF 55 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 310459-07-5 REGISTRY  
CN Deoxymulundocandin, 1-[(4R)-4-[(2-aminoethyl)amino]-N2-[4-[5-[4-(pentyloxy)phenyl]-3-isoxazolyl]benzoyl]-L-ornithine]- (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
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CI COM  
SR CA

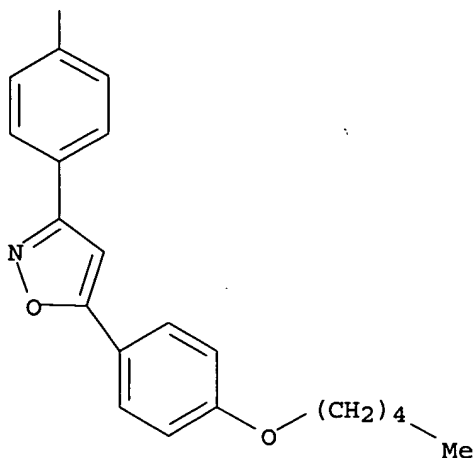
\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.

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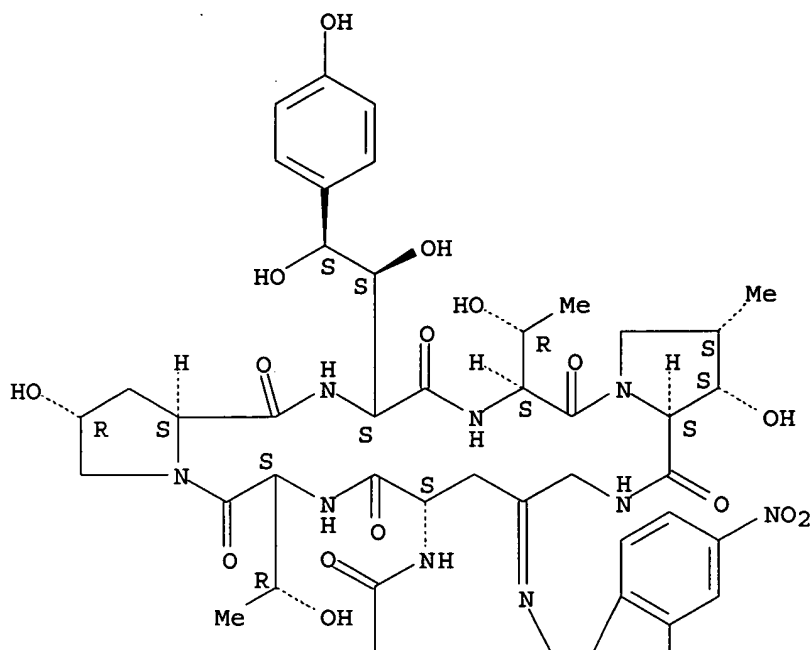
L3 ANSWER 51 OF 55 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 266317-27-5 REGISTRY  
CN Echinocandin B, 1-[4-[(2,4-dinitrophenyl)hydrazono]-N2-[[4''-(pentyloxy)[1,1':4',1''-terphenyl]-4-yl]carbonyl]-L-ornithine]- (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C64 H75 N11 O19  
SR CA  
LC STN Files: CA, CAPLUS  
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RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

**\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\***

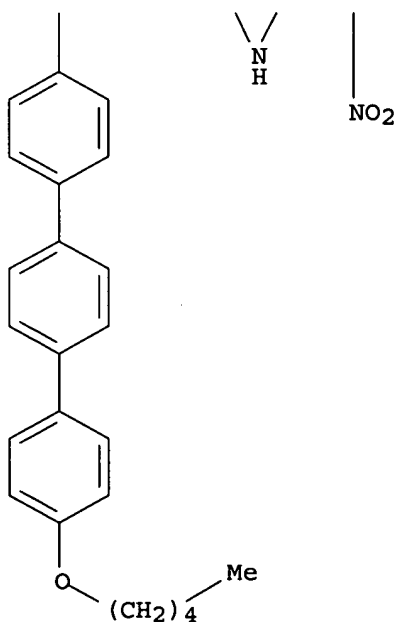
Absolute stereochemistry.  
Double bond geometry unknown.



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1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:308664

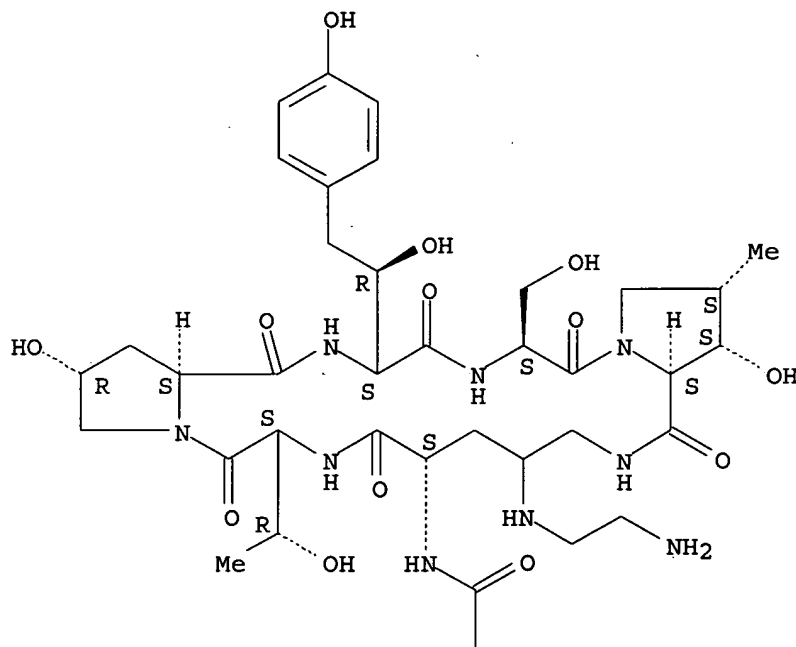
L3 ANSWER 52 OF 55 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 227472-51-7 REGISTRY

CN Deoxymulundocandin, 1-[4-[(2-aminoethyl)amino]-N2-[[4'-(pentyloxy)[1,1':4',1''-terphenyl]-4-yl]carbonyl]-L-ornithine]- (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C59 H77 N9 O14  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA Caplus document type: Patent  
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation)

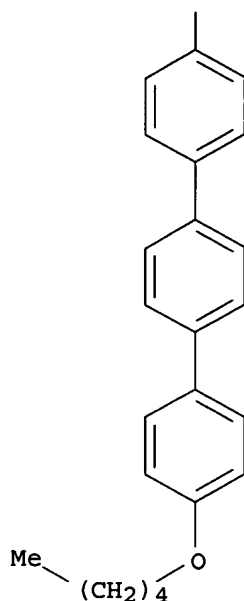
\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.

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1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:45105

L3 ANSWER 53 OF 55 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 227472-50-6 REGISTRY  
CN Deoxymulundocandin, 1-[4-[(aminoiminomethyl)hydrazono]-N2-[4-[4-(4-(pentyloxy)phenyl]-1-piperazinyl)benzoyl]-L-ornithine]- (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C56 H77 N13 O14  
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RL.P Roles from patents: BIOL (Biological study); PREP (Preparation)

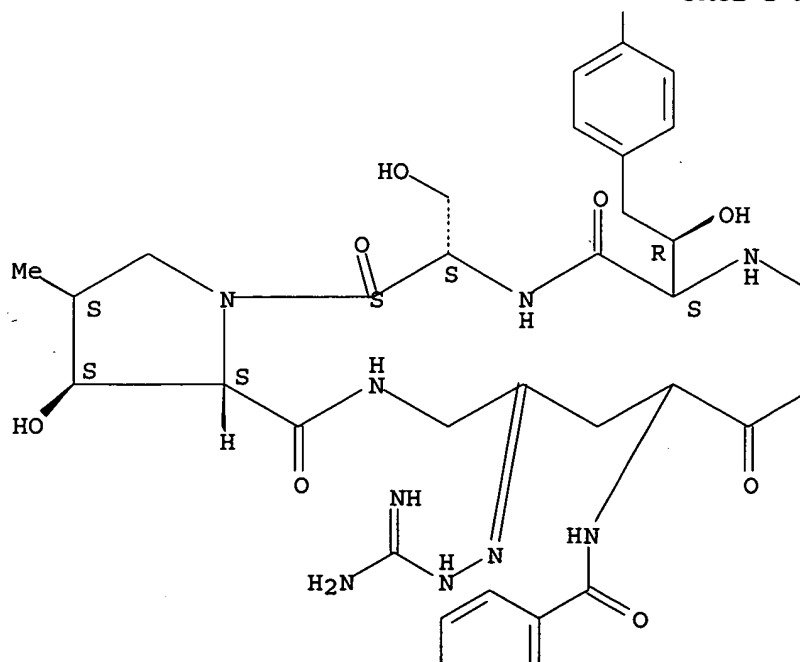
\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.  
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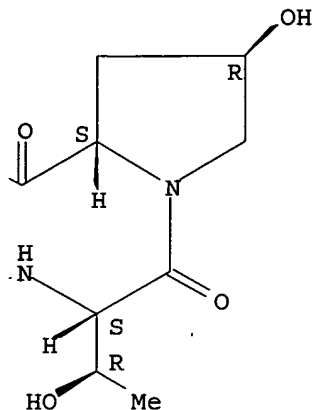
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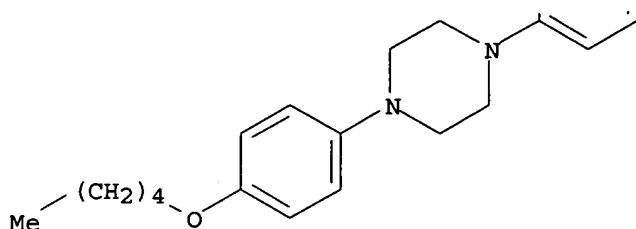
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1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:45105

L3 ANSWER 54 OF 55 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 227472-49-3 REGISTRY  
 CN Deoxymulundocandin, 1-[4-[(2-aminoethyl)amino]-N2-[[4'-(octyloxy)[1,1'-biphenyl]-4-yl]carbonyl]-L-ornithine]-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)  
 FS PROTEIN SEQUENCE; STEREOSEARCH  
 MF C56 H79 N9 O14 . C2 H F3 O2  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 DT.CA Caplus document type: Patent  
 RL.P Roles from patents: BIOL (Biological study); PREP (Preparation)

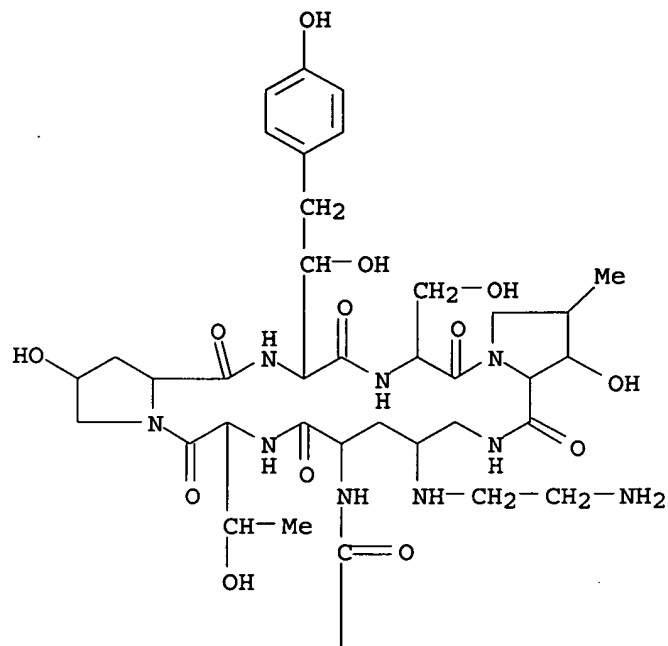
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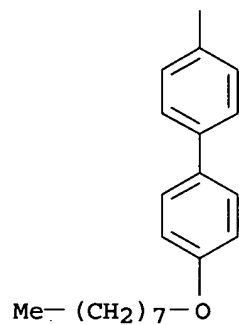
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\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

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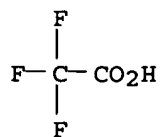
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CM 2

CRN 76-05-1

CMF C2 H F3 O2



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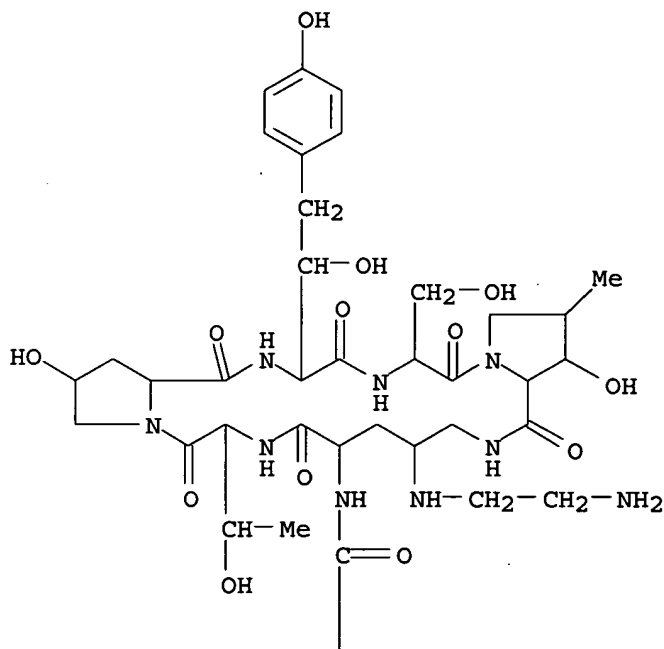
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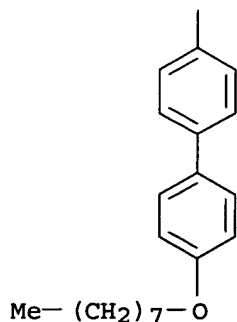
L3 ANSWER 55 OF 55 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 227472-48-2 REGISTRY  
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 FS PROTEIN SEQUENCE; STEREOSEARCH  
 MF C56 H79 N9 O14  
 CI COM  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 DT.CA Caplus document type: Patent  
 RL.P Roles from patents: BIOL (Biological study); PREP (Preparation)

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

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1 REFERENCES IN FILE CA (1907 TO DATE)  
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REFERENCE 1: 131:45105

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